Contents



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NEXT ISSUE OF CRYSTALLOGRAPHY NEWS

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association. Text should preferably be sent electronically as MSword documents (any version - .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (e.g. awards, honours, retirements etc.), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the September 2003 issue are sent to the Editor to arrive before 25th July 2003.

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June 2003

President's Remarks



A novel spin-crossover Material Spinning and Crossing Over

Perutz Prize Lecture

Waterfront Crystallography in York

Hail to the Chief!

Ceremonial and real groundbreaking at Diamond

It is an honour to be writing this, my first column as BCA President. More of that later, but let me start with a few thoughts on the recent Spring Meeting. The York meeting was, in my opinion, excellent, coupling a vigorous and full scientific programme with a great location and organisation. The truncation of the meeting to under three days made us all work hard, and meant few dull moments. Indeed, it is a pleasure to record that any complaints heard by me about the programme were that there was "too much" to be able to attend. A good problem for our Spring Meeting to have congratulations are due to Paul Fewster and the Programme Committee.

It is also a pleasure to note that along with this Crystallography News you should find enclosed a copy of the inaugural BCA Review Symposium issue of Crystallography Reviews. Composed of contributions from last year's Spring Meeting theme "Novel Methods of Phasing", this is the first in what will hopefully become a regular series. Thanks are due to the Crystallography Reviews team at Taylor and Francis, to Moreton Moore, and to the sponsors whose adverts in the issue have enabled us to provide this free to all BCA members. We look forward to the 2003 Review Symposium issue on "High Throughput Methods in Crystallography".

As I said at the top, it is an honour to be elected as President, and a daunting task to follow in the footsteps of a series of highly effective and eminent pastpresidents. It is my intention in my period of office to continue with the increasing professionalism of the BCA, in particular the recent progress made under Mike Glazer and Chris Gilmore, exemplified by the seamless administration of our Association by Northern Networking. Incidentally it is a pleasure to note that our membership

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now tops the 1100 mark. I am aware that we on Council must continue to work together with our membership to maintain the leading position of the BCA in reflecting the strength of our science in the UK, and representing UK crystallography in the world-wide community.

However, I feel we must also reach out to colleagues in structural science who do not necessarily regard themselves as "crystallographers", and increasingly utilise the diversity of our membership's interests to target crystallographyrelated colleagues and attract them along, if not to membership, then to attend our meetings. Underpinning this is the Spring Meeting, which we should continue to develop as the wellestablished annual focus for the whole Association. The Spring Meeting allows us to assemble together and further develop our diverse cross-disciplinary scientific programme. In this era of cross-disciplinarity, the BCA naturally embraces it and can work from this strong position. However, I would stress that to maintain the vibrancy of our subject it is important that we continue to evolve. To use the Spring Meeting as an example, I think it is vital that the topics covered continue to reflect a mix of general interest and specialist topics. Along with the terrific input we already have from the subject groups, I would encourage additional input, for example from Special Interest Groups or colleagues outside the BCA, to ensure that the scientific content fully reflects the challenges being met by our subject today. I would like the job of the Spring Meeting Programme Committee to be a tough one in selecting from lots of excellent session proposals!

I welcome your views and opinions on BCA matters.

Chick Wilson

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2003 - 2004

BCA Council Members 2003 - 2004

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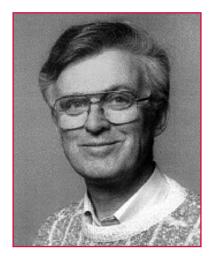
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The British Crystallographic Association is grateful to Birkbeck College, University of London, who host and manage the server for our website: http://bca.cryst.bbk.ac.uk/BCA/ giving access to the BSG, CCG, IG and PCG websites.



From the Editor



The York meeting passed in glorious sunshine, and seemed to be rated a great success by everyone. A warm welcome in particular to our lively new President! Reports of many of the sessions at York are included in this issue. As readers will have noticed, Crystallography News has grown during the past year, and expenditure has exceeded income. We are thus trying to restrict the size of each issue slightly. There has been a particularly bumper crop of good submissions this time, and some of these will appear in the September issue.

Our apologies to Georgina Rosair for advertising her article on service crystallography on the cover of the last issue and then losing it! Unless the gremlins are particularly clever, it should really be here this time. It was good to discover that she was not the only person who noticed that it wasn't there!

We have had several comments about Lachlan Cranswick's article on intellectual patents, and it certainly seems an issue that won't go away. As I write this, I tune in from time to time for the latest riposte in the ongoing exchange between Alan Hewat and Armel Le Bail (and an increasing number of others) on the rietveld network over access to databases. It makes stirring reading, and anyone not connected to rietveld_ l@ill.fr has been missing an elegant debate!

Meantime, intellectual rights issues have touched another of our own ongoing subjects. "Bars, the boring kind", to use Mike Hart's name for those annoying little lines we put over numbers, continue to generate mail! Tony North wrote about a scheme he has for barring numbers, but it seems that it is hush-hush for the time being, as it is to appear in an article by Tim Nott in the July issue of Personal Computer, so don't miss that! Hopefully, after July the technique will be freely available for use without royalty.

Crystallography News has a wider readership than we thought! We have received a communication from Dr Paul Hartal of Montreal about the mention of his article The Songs of the Double Helix: Symmetry and Lyrical Conceptualism in Kate Crennell's review of Hargittai and Laurent's Symmetry in last September's Crystallography News (page 19). Kate and I both apologise for misspelling his name and for being uncertain about the seriousness of his concept of "lyrical conceptualism". Readers who wish to know more about this approach to the relationship between science and art are referred to the website: http://www.arthbys.com/Paul_Ha rtal.htm for further information.

Bob Gould May 2003

Stop press: New Fellows of the Royal Society

We are very pleased that three of our members have been made Fellows of the Royal Society this year. They are Professor Eleanor Dodson, Research Fellow at York, Professor Richard Nelmes, Professor of Physical Crystallography at Edinburgh, and Professor Venkatraman Ramakrishnan, Senior Scientist, MRC Laboratory of Molecular Biology, Cambridge. Our heartiest congratulations to all three. Full citations may be found on the Royal Society Website: http://www.royalsoc.ac.uk/.







Charging for Services

June 2003

Charging for X-ray Crystallography services

University administrators are becoming more determined to balance the books in all areas of university life, so university activities are put under pressure to be "value for money" and pay their own way. The analytical services in my department have been asked to come up with a charging scheme for the work we do. The challenge is to find a system that is fair but not overly complex to administer. In October, I put out a questionnaire on the BCA Chemical crystallography group website (thanks to Harry Powell for setting it up) and posted it to the sci-techxstallography news group. In all, I received seven replies: 4 from the UK and 3 from the US. The questions asked were:

- Do you make a charge to research supervisors for crystal structures obtained by

 a) service personnel or
 b) amateur operators?
 If so, what is the charge? (E.g.
 How many pounds per structure, pounds per hour etc.)
- 2) Where does the money go?(Does it go into general departmental or university accounts, or is it all kept by the crystallography service?)
- 3) How is the crystallography service paid for? (E.g. do you get a grant or budget from the department or the university to cover costs? Do you use only the income from service charges? Is it some combination of these?)
- 4) What expenditure is permitted (or required) from the income you receive? Can you say what the situation is for the following types of expenditure:

- a) Salaries of crystallography service personnel - or are these paid by the university or department?
- b) Consumables e.g. cryogens, paper, etc
- c) Repairs in total, or below a certain limit?
- d) Equipment upgrades is this subject to any annual, or item limit?
- e) Is it restricted to accessories only, or may/must you buy other items too?
- 5) Equipment renewal i.e. the next new diffractometer.
- Any other categories you might have! - e.g. travel and conferences, space charges, phone or photocopying charges.
- 7) Can you retain unspent funds for the next financial year, or is your money zeroed at the beginning of each year?
- 8) What happens to fees or charges received in respect of commercial or consultancy work?

The situations in the UK and the US are very different. Many UK respondents didn't charge for departmental work, but some of these expressed concerns that they may asked to do so in the future. All UK services were funded to some degree by their university departments. Those that did not charge for their work were financed from top slicing of the department budget. All US labs that responded did charge for work.

Most UK labs charged a flat rate per sample but one lab divided the charge according to the amount of work required on the sample. The structural analysis was divided into three areas: crystal screening, data collection and structure solution/refinement. The crystal screening charge allowed for 3 samples to be screened, thereby discouraging poor quality crystals from being submitted, when better crystals could be obtained by regrowing them. The charge for data collection covered up to 24 hours. Thereafter it was one unit per 24 hours. If the structure was solved and refined by the chemist or colleague, even with major help from service personnel, no charge was made for solution/refinement. If service personnel did this part as well, the charge was doubled. This system was the most complex described, yet it was built to encourage students to get good crystals and to learn to solve and refine their own structures.

In the US, services which had to be self-sufficient (bar staff salaries) charged substantially more (\$300 per sample), than those with more financial support from their departments (\$150). In both these cases, when the work was carried out by chemists doing their own crystal structure analysis, there was no charge. Another US facility charged per hour. There were 2 charges, one for instrument hire per hour and a second charge for service personnel time per hour. Therefore, chemists doing their own crystal structure analysis were charged for instrument use alone.

University departments paid for salaries in both UK and US cases. Some personnel were paid for from research grants but none were paid from the service income. Department accounts paid for repairs and inexpensive accessories, but large capital investment such as new diffractometers were bought with money from grants. X-ray tubes were bought from

Charging For Services

CCG AGM

accumulated service income or from special department funds for repairs and replacements.

At the end of the financial year, the service accounts were zeroed (usually for departments who didn't charge) or carried over into the following year, if there was a surplus which could be accumulated to fund a large purchase.

Income from commercial work generally went into a service account, but part of the income was taken by the university or department. Occasionally, some of the income went directly to the service personnel through their salary.

Some of these procedures may work well for your lab, others would need to be adapted. Charging for crystallography in a university department is a balancing act and many of us would prefer not to have to charge at all but to choose to do the work on basis of scientific merit rather than income. In the current climate we may not have a choice.

Thanks to all those who replied to the questionnaire. If you have not replied to the questionnaire, and particularly if you have additional comments on managing an x-ray service, please e-mail me G.M.Rosair@hw.ac.uk

Georgina Rosair



The author at a multicircle site in Scotland

Spring Meeting: CCG AGM

There were a number of items of general interest to the Group which arose during the CCG AGM held at York on 16th April; the Group now has a new Chairman and Deputy Chairman, as well as a new Committee member and co-opted Student Representative. We also have a slightly amended Constitution. The Minutes of the Meeting will be available at a later date.

There were 46 members present at the AGM.

The current members of the Committee (with terms of office) are:

Chairman: Sandy Blake (Nottingham) 2003 - 2005 Deputy Chairman: Simon Parsons (Edinburgh) 2003 - 2005 Secretary/Treasurer: Harry Powell (Cambridge) 2000 - 2004

Committee:

Simon Coles (Southampton) 2001 - 2004 Richard Cooper (Oxford) 2002 - 2005 Michaele Hardie (Leeds) 2002 - 2005 Mary Mahon (Bath) 2003 - 2006 Georgina Rosair (Heriot-Watt) 2002 - 2005 Simon Teat (Daresbury) 2002 - 2005

Co-opted Student Representative: Katharine Bowes (Cambridge) 2003 - 2005 Co-opted 2003 Autumn Meeting local organizer: Vanessa Hoy (Accelrys) 2002 - 2004

Sandy Blake and Mary Mahon were elected unopposed, while Simon Parsons won in a close contest with Chris Cardin (Reading). Those of us who had anything to do with CCG

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activities over the past few years will want to thank the retiring Chairman (Paul Raithby), Committee member (Jon Steed) and Student Representative (Duncan Tooke) for all their contributions.

The Constitution was amended to allow a single officer to sign cheques for the CCG bank accounts rather than requiring two signatures. The proposal to allow this was passed by a unanimous vote of the AGM; notice of this proposed change to the Constitution was circulated by e-mail to the Group one month before the AGM. The revised Constitution may be seen on the CCG website.

Coincidentally with this, it was agreed at the AGM (again by a unanimous vote) that the Group's bank accounts should be moved to the Charities Aid Foundation bank, CAFCash Ltd. This move will give higher rates of interest than available with the Group's current banks, and also streamline transfers between current and deposit accounts.

Finally, a plea from the Secretary! If you don't receive e-mail circulars from the CCG, or know of anyone else who should get them but doesn't, please let me know

Harry Powell



Poster Prizes

Industrial Group

Spring Meeting: CCG Poster Prize Report

The CCG Poster Prize for 2003, generously sponsored by Oxford Diffraction, was won by Amber Thompson of the University of Durham. Her poster entitled "STRUCTURE-PROPERTY CORRELATIONS OF NOVEL SPIN CROSSOVER MATERIALS" was commended for its high scientific content and visual impact. It is the result of a collaboration between Durham and Valencia. "When these spin crossover



materials are heated, or placed under vacuum, they lose ligated water and the free nitrogen of the pyrimidine ring moves to occupy the coordination site. This process is completely and swiftly reversible, and is unusual as it is a major structural change that takes place in the crystalline state."



Cheryl Doherty (Bath) gained an honorable mention for her poster "X-RAY DIFFRACTION STUDY OF PHENOL: RADICAL ADDUCTS: A STRUCTURAL MODEL FOR H-ATOM ABSTRACTION BY PEROXYL RADICALS FROM VITAMIN E".

Francesca Fabbiani (Edinburgh) won the Industrial Group Poster Prize for her poster entitled "HIGH-PRESSURE ROUTES TO NEW POLYMORPHS AND SOLVATES OF ORGANIC MOLECULES".



Industrial Group

Following the AGM at York, the Illustrious members of the BCA Industrial Group Committee, enjoying the Spring Meeting 2003 were as follows



From left to right, Back row Neil Feeder, Phil Holdway (News Letter Editor...hiding!) Chris Frampton (Chairman), Richard Morris, Mark Farnworth In the front Jeremy Cockroft (Vice Chair), Judith Shackleton (Secretary/Treasurer), Brett Cooper.

Escapees from the camera David Beveridge, Steve Norval & Dave Tayor (ICDD Representitive)

Industrial Award 2002

During the November Meeting of the Industrial Group, the latest in the series of Industrial Group Awards was given to Jo Jutson, Editor of Crystallography News in 2001, to mark her service to the BCA and her helpful involvement in the wider scientific community. Chris Frampton gave a short address, reviewing Jo's scientific career and contributions. (He omitted to note that this has included scientific presentations to her WI Branch: I wonder if this is unique among recipients of the Award?) Chris invited Jo to give her paper "From Spinel Analysis to Micro X-ray Diffraction - a Personal View of Applications and Advances" which she did with her characteristic modesty and clarity. In the picture, Jo is receiving a Beevers Model of spinel from Chris Frampton.



Obituary

June 2003

John H. Robertson 1923-2003

John Robertson was brought up in China where his parents were Christian missionaries. [In 1980 he claimed to know no Chinese "We were not allowed to talk to the servants".] He attended the University of Edinburgh and graduated in chemistry in 1946. He then began work on a Ph.D. under the supervision of C.A Beevers. These were the first days of the determination of absolute configuration, with much friendly rivalry between Arnold Beevers and J.M. Bijvoet in Utrecht, both of whom worked on salts of strychnine. John studied the chloride, bromide and iodide salts, and his beautifully developed and labelled normal-beam Weissenberg photographs are still preserved in Edinburgh. He solved the structure of the bromide, in P212121, on the basis of the three projections and then refined in three dimensions to determine the chirality. Happily, the Bijvoet group determined the same hand for the selenate salt! Meanwhile, the samples also survived, and the structure of the chloride, which gives pseudoorthorhombic monoclinic crystals with Z' = 2, was solved by one of us (ROG) in 1980, using John's crystals. Sadly, COSHH regulations eventually resulted in their disposal!

From 1951-54, John had a happy post-doctoral period in Dorothy Hodgkin's group working on, the SeCN and the hexacarboxylic acid derivatives of vitamin B12. He has described this period in Memories of Dorothy Hodgkin, Structural Studies of Molecules of Biological Interest, Ed. G.Dodson, J.P .Glusker and D.Sayre (1961) 72-78. In 1954 he joined E.G.Cox's group in the University of Leeds. Here, he used his great experimental skill to build an instrument to allow X-ray photographs to be taken of a crystal at the temperature of liquid hydrogen, and used it to study ammonium oxalate monohydrate. MRT remembers working on it with him one day and seeing nonmatching earrings when she got home. She teased him with failure of observation. Quick as a flash he said "I did notice, but as it was you, I thought it must be the dernier cri !" Later he undertook the neutron study of this elegant compound. Various thoughtful publications followed, on oxalates, thiophenic acids, monosaccharides and coordination compounds of iron and nickel. Apart from a period (1965-68) on secondment as the founding Professor of Chemistry in the University College of Dar-es-Salaam, he remained in Leeds for the rest of his life. He was promoted to Senior Lecturer and various Heads of Department did not allow him to take early retirement because, being totally unselfish, he was much too useful. For example, he ran the Colvin Room, a common room and library for chemistry students of Leeds University. He served the IUCr as an excellent Book Review Editor for its iournals from 1975 to 1987. He then became Chairman of the IUCr-OUP Book Series Committee from its inception in 1987 until 1996, well after his fiscal retirement. His experience as a sandy-haired person in the sun showed at the 1969 IUCR meeting when the conference excursion took the form of 5 hours on an Atlantic beach on Long Island. As we were warned in the coaches on the way, this is the latitude of Madrid. Walking along the shore was an unmistakable figure in hat, mackintosh, trousers and shoes. His last years were saddened by the long illness of his very dear wife Inge, which prevented him travelling, and after her death by his own incapacity.

Many people will remember him as a widely-read and civilised person with a very lively sense of humour, shared with his Ph.D. supervisor Arnold Beevers, with whom he remained on good terms throughout his life. He gave a memorably uproarious lecture at Arnold's 70th Birthday celebration in 1978, and the photograph was taken ten years later at the 80th birthday party. He was always very fond of children. ROG's daughter remembers him as "the man at crystallography meetings who drew cats on my knees." His sincere but undogmatic Christian belief was the guiding spirit of his life; a typical example was that his Christmas cards always consisted of photographs of his family with a montage of 'Peace and Joy'. We conclude with an extract from the passage he wrote to be used at his funeral:

"All life is finite. This is the way God designed the natural order. Successive generations are cradled in the arms of their forebears. We ourselves would not be here if death, as well as life, were not normal throughout the whole of nature. To be sure, human life is special. We can feel God's love for us and can respond and so live in a dimension infinitely rich and profoundly significant."

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We are grateful to Prof. D.W.J.Cruickshank for helpful information.

Jackie Truter (MRT) and Bob Gould (ROG)



John and Inge Robertson.

Harry Francis West Taylor (1923 - 2002)

H. F. W. Taylor, energetic, forthright and an enthusiastic supporter of careers for women long before this became PC, was always known as "Hal" to his colleagues and friends. His scientific career spanned over fifty years and saw great changes in crystallography, from home-made equipment and Beevers-Lipson strips to automatic diffractometers and high-powered computers.

He began his studies at the University of Nottingham, and subsequently moved to Birkbeck College, London (1948 -1953), which provided a uniquely stimulating environment, in large part due to the presence of the late J D Bernal. While there, he worked on a range of topics using methods and equipment that were incredibly primitive by today's standards. He used to recount that his introduction to crystallography commenced by being told by Bernal to build his own film cassette for a single crystal camera (on the lines of a Unicam S25 - and how many modern crystallographers have used one of those?) from a tin can and bicycle clips.

In 1953, he was offered a permanent post in the Chemistry Department at Aberdeen University, where he remained until his formal retirement. On arrival there, his interests turned to mineralogy and the crystal structures of the naturally occurring calcium aluminate and silicate hydrates, especially as a route to elucidating the structures of the poorly-crystallised cement phases. In addition to solving many crystal structures by x-ray crystallography, he quickly realised the potential of electron microscopy and diffraction. With the late Dr. J. A. Gard, he solved mineral structures for which only poorly-crystallised or disordered minerals or fine-grained synthetics were available.

At this time, Hal also became interested in topotactic reactions in various structures, particularly silicates; I was one of his first research students, and was privileged to work with him on this. He was a stimulating supervisor, and during that time we following the string-and-sealingwax tradition - built apparatus to do the work and succeeded in studying a number of mineral transitions.

The advent of automatic diffractometers and high-powered computers opened a new world to Hal, as it did to the rest of us. No longer was peering at spots on film to gauge their intensity followed by laborious calculations: Hal seized on the advances with gusto, and became an enthusiastic computer programmer.

Hal was an excellent and inspiring supervisor; he never had many students at any one time but those whom he took on were intensively trained and actively encouraged to present papers at meetings. His enthusiasm for crystallography was unbounded and he gave unstintingly of his time and intellect to others, often without seeking acknowledgement of his contribution. He regularly attended crystallography meetings, both national and international, and I remember many stimulating discussions arising from these. He served on the committee of the Crystallography Group of the Institute of Physics (before the days of the BCA!).

Hal contributed also to undergraduate teaching, assuming a full share of lecturing, tutorials and laboratory work, including the most difficult assignment: lecturing on chemistry to the elementary classes, including those taking chemistry as a necessary option, whose motivation presented a significant challenge. His highly successful scheme for the organisation of the laboratory classes persists to this day with but slight modification.

Hal was a clear and careful writer, and was frequently asked to write books and articles. He edited a multi-authored two-volume book on cement chemistry, which appeared in 1964. Writing his own book on the subject had to wait until later, but the first edition (1990) and fully revised second

Obituary

Book Reviews

edition (1997) have probably become the most widely read single text on cement. The book has been translated into several languages and, moreover, several pirate editions - perhaps the ultimate accolade of a successful science book - were also made!

Hal served a term as head of department, 1977-1980, conscientiously but without great enthusiasm; administration held no charms for him, and it was increasingly a time of stringency and retrenchment within the University. After the completion of his headship in 1980 he took partial and later full retirement from Aberdeen, to pursue research and writing. A series of honorary Professorships followed, first at the Imperial College, London and subsequently at Leeds. This was a happy period: he could continue to guide students while remaining largely free from administrative duties.

Formal retirement also meant more time for mountaineering a lifelong interest that began in Wales and subsequently encompassed all the Scottish mountains and many of the European alpine peaks as well as others in the Americas, Asia and Africa. He remained in excellent physical condition until late in life, when increasing heart trouble forced an operation. Initially successful, the benefits of the operation gradually diminished. However he remained professionally active and only succumbed - guite suddenly - while journeying home from a meeting abroad. This was what Hal would have



wished: he never had to experience a long drawn out period of invalidity.

Hal's career attracted many honours and distinctions. He was on the editorial boards of numerous journals, and was a Fellow of many organisations including the Royal Society of Edinburgh. He received the Kroll medal and prize of The Institute of Materials and The Copeland award of The American Ceramic Society amongst many distinctions.

We shall remember him for his unbounded enthusiasm and zest for life, his inspiration of students and colleagues, generosity in sharing ideas, and on a personal level - his wonderful down-to-earth sense of humour. We miss him greatly.

He is survived by his wife, Joan, and a son, Robin, to whom we extend our deepest sympathies.

Lesley Dent Glasser

Crystal Growth Technology

K. Byrappa and T. Ohachi (Editors) William Andrew Publishing, New York and Springer Verlag, Berlin, 2002

Price: US\$ 155 (hardback) or £105 ISBN 0815514530; xxi + 590 pages.

Crystal Growth Technology is a commendable addition to the extensive literature of crystal growth because it aims to cover techniques and processes in current use for the production of industrially important crystals. Single crystals are the foundations of modern industry but, despite their enormous economic importance, details of production processes are sparsely represented in conferences or in the literature. (It should be noted that the first international school on crystal growth technology as a specific topic was not held until 1998). The editors of the book, K.Byrappa and T. Ohachi, are distinguished workers in the world of crystal growth, Byrappa in hydrothermal growth and Ohachi in molecular beam epitaxy. The book has seventeen chapters, only two of which (Chapters 2 & 8) are exclusively theoretical, each being a review of some topic related to the production of industrially and biologically important crystals.

Reviewing a book compiled from contributions by a number of authors requires two interlinked approaches, one of which, in common with any other review, is an assessment of the success of the book in meeting the specification implied by its title, the other being the discussion of the merits of individual contributions. In case of

Book Reviews

the present book, individual chapters can hardly be faulted. Indeed, it is unusual for all the contributions in such a compilation to be of such a uniformly high standard and the editors are to be congratulated. An analysis of every chapter would make this review intolerably long but a few have been selected for more detailed discussion.

Ichiro Sunagawa's subject (Chap.1), morphological features of mineral crystals, may seem a surprising choice for inclusion in this book but the author's extensive knowledge and deep understanding of crystal growth have resulted in a stimulating essay on the significance of morphological features, which, despite the examples being restricted to beryl, diamond and ruby, is of much more general significance, and should be important even to workers studying the growth of crystals in a biological environment.

Irisawa's contribution (Chap.2) on the theory of crystal growth from vapour and solution is a competent treatment of basic theory starting from the concept of thermodynamic driving force and the surface models of Kossel and Stranski. The treatment is extended to growth from solution and incorporates the necessary modifications of the theory to cope with solvation effects. The chapter is well presented but is essentially introductory and covers only longestablished theory. I feel that most potential readers of this book will be already familiar with theory at this level or, at least, have access to more comprehensive and recent work.

Molecular beam epitaxy (MBE) has evolved from being a powerful research tool into a technique for the production of specialised nanostructures in III-V compounds and the parallel development of vapour-phase epitaxy using organometallic compounds (MOVPE) has resulted in important new optical and electronic devices. The chapter by T. Nishinaga and S. Naritsuka (Chap.3) provides a compact review of both these processes and emphasises the fact that the purity level achieved by MOCVD is not inferior to that obtained by MBE. The chapter is divided approximately into three, the first two parts covering MBE and MOCVD and comparing their chemistry and elementary growth processes. The final part describes the production of nanostructures such as quantum well wires (QWW) and quantum dots. This part also covers highly mismatched heterogeneous interfaces and the production of GaN lasers by microchannel epitaxy.

The chapters on diamond synthesis (4), silicon carbide (6 & 7) and quartz (11) strike an excellent balance between basic science and practical details. All these chapters have extensive lists of valuable references.

Chapter 16 is an admirably detailed review of the growth of hydroxyapatite crystals related to biomaterials. Calcium orthophosphates, particularly hydroxyapatite, occupy an important place in many biological and medical topics: they are associated with pathological calcifications such as dental plaque, urinary calculi and artherosclerosis; they form the foundations of bone and tooth structures and they find use as orthopaedic and dental cements. The authors, Atsuo Ito and Kazuo Onuma, introduce the calcium orthophosphate family and discuss the prevention of undesirable calcification at the surface of implanted biomaterials, the composition and properties of phoshate cements and the various factors influencing the formation of hydroxyapatite in hard tissue. These diverse processes are shown to depend entirely upon the crystal growth kinetics of hydroxyapatite. This chapter provides an extremely informative review and, with its 196 references, is an approachable and comprehensive introduction to this important and growing field.

The last chapter (17) is devoted to the growth of gemstones and is a good general review of the subject but does not present much new information and would have been more appropriate in a gemmological publication. In view of the two outstanding chapters on silicon carbide already referred to, it seems strange that this chapter makes no mention of recent work on the important SiC gemstone, moissanite. (See, for example, K. Nassau, J. Gemmology, vol. 26 [7)] 1999).

The chapters not individually discussed cover the following topics: laser-assisted growth of PZT films, multicomponent perovskites, borate crystals for non-linear optics, hydrothermal growth of rare-earth vanadates, lithium niobate & bismuth germanate, hightemperature superconductors and zinc chalcogenides.

Considered as a whole, the book is successful in presenting compact

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and well-written pieces on selected topics. However, it does suffer from the omission of some extremely important subjects, for example, silicon, scintillators, habit control in bulk crystallization, corundum, large-scale growth from aqueous solution, and organic compounds. While no book can be fully comprehensive, I feel that, if some of these gaps had been filled, it would have been a more satisfactory piece of work. The aims of the book would have been achieved to a greater extent also if the amount of background science had been reduced and more emphasis given to contemporary production methods. Some of the chapters, although of good quality, might have appeared in any conventional book on crystal growth with no claim to a particular emphasis on technology or production.

This book would certainly be a desirable addition to a library but, with the price set at £105, it cannot be seriously recommended to individual purchasers.

As a result of reading this book although this is not intended as a criticism - I have been reflecting on the current use of the word technology and would like to make a plea for some restraint. The word technology meant originally the study of science applied to industry but in the last 20 years or so it has been battered almost out of recognition. Politicians, journalists and other scientific illiterates tend to use the word when they refer to anything involving computers, while the scientific community use it indiscriminately as a fashionable blanket term so that they can avoid making the small effort needed to

decide whether they mean method, technique, process, equipment or procedure. Perhaps we should all hesitate the next time we are tempted to say or write anything about technology.

Peter Dryburgh University of Edinburgh

Intimate Triangle: Archtecture of Crystals, Frank Lloyd Wright and the Froebel Kindergarten

Jeanne Spielman Rubin Polycrystal Book Service, 2002 Price: \$44.95 (hardback) ISBN 0971877602; xvii + 329 pages.

I've sometimes wondered whether infiltrating children's playgroups with building blocks of all seven crystal systems would build a nation of crystallographers. It would certainly seem from reading this book, that early Froebel training in spatial awareness strongly influenced Frank Lloyd Wright (1867-1959) and many other notable architects, artists and thinkers: including Le Corbusier, Paul Klee, Piet Mondrian, Maurits Escher and even Albert Einstein.

Interestingly, the author is an emeritus professor of music, who lives in a house specially designed for her by Frank Lloyd Wright. FLW's mother apparently discovered Friedrich Froebel's system of education when she visited the Philadelphia Centennial Exhibition in 1876. His father (William Russell Cary Wright) was superintendent of schools in Richmond County, Wisconsin as well as an accomplished musician, who felt that music was the closest art to architecture, in form, structure and ornamentation. FLW's early years were spent listening to his father playing Beethoven on the piano and playing with Froebel 'gifts' provided by his mother.

Friedrich Froebel's life of educating (1782-1852) overlaps with that of Heinrich Pestalozzi (1746-1827) and comes a century before Maria Montessori (1870-1952). His system gave the elementary geometrical basis for design and awakened the child mind to 'rhythmic structure' in Nature by the use of constructive playthings (the 'gifts') presented in a specified order. It seems very likely that Froebel's interest in geometrical ideas was reinforced when he became Assistant at the Mineralogical Museum of Berlin, working under the guidance of Christian Samuel Weiss (1780-1856) - the Weiss of the zone law. He was later (1816) offered the professorship of mineralogy at Stockholm University, an invitation which he appears not to have taken up; but his nephew, Julius Froebel, did become Professor of Mineralogy at Zürich.

The Froebel education scheme consisted of the 'gifts' – cubes, spheres, cylinders, cones and many other things – together with the 'system'. The latter embraced the Froebel laws of unity, contrasts, development and connections. Nature observes natural laws when creating, so humankind should also follow them in creative endeavours.

The longest chapter (of over a hundred pages) gives details of all the 'gifts' and the possible connections with FLW's architecture and with geometric crystallography. Several examples are given of four-

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fold rotational symmetry exhibited by FLW ground plans. There are clear similarities between the nets/meshes drawn on the Froebel table and two-dimensional crystallography. The solid shapes of the cone, cube and sphere were considered by Cézanne to be basic to all others. To these basic shapes, Le Corbusier added the cylinder and FLW the tetrahedron. There are parallels between illustrations in Owen Jones's famous architectural textbook The Grammar of Ornament (1856) and the symmetry groups of crystallography. Arrangements of Froebel's bicoloured tablets find complete expression in the dichromatic space groups of Shubnikov and Koptsik (1972).

Although R Buckminster Fuller attended kindergarten, it is not entirely clear whether he was Froebel trained. He was once introduced by FLW as 'a scientist interested in architecture', whereas FLW described himself as 'an architect interested in science'. Fuller apparently was visually handicapped to the point of being legally blind from birth: before being fitted with spectacles he had gained his three-dimensional insight through tactile awareness. Certainly he had a great gift for designing structures from tetrahedra and octahedra, and huge polyhedral domes.

I cannot say that this is essential reading for every crystallographer, but if anyone wishes to pursue the connection between early kindergarten training and eventual profession, this book provides many of the clues. It is a scholarly work, with over 150 references, 360 notes and a good index; and it contains many interesting historical anecdotes tracing the influence which members of the various connected families in the USA, Germany, Italy and Switzerland had upon educational reform.

Moreton Moore

International Tables for Crystallography, Volume E: Subperiodic Groups

V. Kopsky and D.B. Litvin, Editors IUCr/Kluwer Academic Publishers 2002 Price: £150.00(full rate), £75.00(reduced rate) (hardback) ISBN 1402007140 ix + 562 pages.

Volume E is the fifth of the "New" International Tables to appear. It covers subperiodic groups, that is, those which are periodic in one or two dimensions and finite in the others. It is composed much in the style of Volume A, with large, clear diagrams, and most of the same tables, including general and special positions, projections and sub- and supergroups. While it will certainly not command the market that Volume A does, it is almost certainly of greater relevance than it may seem to the average crystallographer, as so many structures may be considered as built up from substructures having the symmetries described here.

After an introductory chapter, the first symmetry groups covered are the 2 oblique and the 5 rectangular frieze groups (2-dimensional overall, periodic in one dimension). As these relate to the 17 plane groups, they provide a good introduction to the much more complex rod and layer symmetries which relate to three dimensional objects.

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The next section gives the 75 rod groups (3-dimensional overall, periodic in one direction.) Unlike friezes, rods may have an axis of any dimension along the rod, and the authors necessarily include only those which can arise from crystallographic symmetry. Diagrams for the higher symmetry rods show the projection along the rod axis only, while the 22 groups deriving from orthorhombic or lower symmetry show the three projections. Oddly, the projection along the rod is invariably shown as a circle, although an ellipse would seem more suitable, as such rods do not require circular cross-sections.

The third set of groups, the 80 layer groups, are 3-dimensional overall and periodic in two of these. In these diagrams, only the projection along the non-periodic direction is given.

The final section of the book gives scanning tables, where scanning is defined as description of the spatial distribution of local symmetries. In this case, those of interest are the penetration rod groups and the sectional layer groups. Well laid-out scanning tables are given for each of the 230 space groups, and the various sectional layer groups are given explicitly. However, the "distribution of the penetration rod groups is seen directly from the scanning groups" and this is less convenient, as the order and naming of some elements has to be changed.

Examples are given of the uses of the groups, particularly for well known layer structures such as cadmium chloride, and for twin junctions. The contents of the book must, however, also be recommended to molecular and macromolecular crystallographers who encounter the same penetrating rods and sectional layers.

Bob Gould

June 2003

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2002.

Examining Accountant: R A Young, BSc. FCA. The Young Company, Lakeview Court, Ermine Business Park, Huntingdon PE29 6XR These are consolidated accounts and include the BCA, BSG, CCG						
and IG funds and are expressed in pounds sterling (£) INCOMING RESOURCES:						
	2002	2001				
Grants and sponsorship	(328)	19,237				
Donations	2,240	1,206				
Annual conference	65,142	59,481				
Meetings of groups	2,988	3,843				
Newsletter	27,231	23,797				
Membership subscriptions	16,020	14,380				
Course fees	-	15,521				
Net income from trading	(2,369)	16				
Investment income	6,097	5,419				
Interest received	1,498	2,929				
Glasgow 1999	-	32,114				
Sundry income	-	277				
TOTAL INCOME	118,519	178,220				
EXPENSES:	2002	2001				
Direct charitable expenditure (1)	97,093	141,918				
Management and administration (2)	19,379	18,090				
TOTAL EXPENDITURE	116,472	160,008				
	2002	2001				
NET INCOME	2,047	18,212				
Unrealised gains (losses) of investment assets	(6,144)	(2,895)				
NET MOVEMENT IN FUNDS	(4,097)	15,317				
Balances brought forward at 1 January 2002 Balances carried forward at 31	194,221 190,124	178,904 194,221				
December 2002	190,124	1)4,221				
ASSETS: Fixed Assets	2002	2001				
Tangible assets	1,037	36				
Investments	91,209	94,386				
	92,246	94,422				
Current Assets	2,210	91,122				
Stocks	743	3,240				
Debtors	5,691	17,556				
Cash at bank	102,252	96,563				
	102,252	117,359				
	108,080	117,339				
LIABILITIES: amounts falling due within one year	(8,970)	(15,793)				
LIABILITIES: amounts falling due after more than one year	(1,838)	(1,767)				
NET ASSETS	190,124	194,221				
INCOME FUNDS:	2002	2001				
Restricted funds (3)		62,783				
	63,848	<i>'</i>				
Unrestricted funds (3)	126,276 190,124	131,438 194,221				

NOTES TO THE SUMMARY FINANCIAL STATEMENTS:

1. DIRECT CHARITABLE EXPENDITURE

	2002	2001
Previous year conferences	8	548
Subscription to International bodies	3,492	1,925
Annual conference	57,988	59,052
Meetings of groups	331	1,330
Newsletters	29,147	20,247
Course fees and accommodation	-	29,962
Grants and sponsorship	500	2,050
Prizes	627	160
IUCr Congress	-	25,000
Arnold Beevers Bursary Fund	4,000	1,400
Bursaries from restricted funds	1,000	244
	97,093	141,918

2. MANAGEMENT AND ADMINISTRATION

General expenses		
Depreciation	340	45
Administration fee	13,186	13,094
Accounting fee	2,262	2,115
Insurance	368	192
Bank and security charges	190	154
Spring Meeting Planning	34	684
Special Interest Group administration	546	700
Council members' expenses	924	377
Officers	636	447
Other Council expenditure	893	282
Total	19,379	18,090

ACCOUNTING POLICIES.

These summary financial statements are based on financial statements which have been prepared under the historical cost convention, with the exception of investments which are included at market value. The financial statements have been prepared in accordance with the Statement of Recommended Practice, "Accounting and Reporting by Charities" published in October 2000 and applicable accounting standards.

All incoming resources are included in the Statement of Financial Activities when the charity is legally entitled to the income and the amount can be quantified with reasonable accuracy. All expenditure is accounted for on an accruals basis and has been included under expense categories that aggregate all costs for allocation to activities. Investments are stated at market value at the balance sheet date.

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided at rates calculated to write off the cost of fixed assets, less their estimated residual value, over their expected useful lives. Stocks are valued at the lower of cost and net realisable value after making due allowance for obsolete and slow-moving stocks.

The full BCA accounts for 2002 are available on request as an E-mail attached PDF file from the BCA admin office.

The British Crystallographic Association

Summary Financial Statements for year ended 31 December 2002.

3. STATEMENT OF FUNDS	Brought Forward	Incoming Resources	Resources Expended	Gains/ (Losses)	Carried Forward
UNRESTRICTED FUNDS					
General fund	131,438	110,724	109,742	(6,144)	126,276
RESTRICTED FUNDS					
Arnold Beevers bursary fund	19,756	1,951	4,000	-	17,707
Dorothy Hodgkin prize fund	6,120	571	-	-	6,691
Chemical group teaching school	10,068	(1,596)	157	-	8,315
Chemical group fund	2,432	1,786	-	-	4,218
Industrial group fund	7,351	347	1,458	-	6,240
Biological structure group fund	17,056	4,736	1,115	-	20,677
Subtotal	62,783	7,795	6,730	-	63,848
Total of Funds	194,221	118,519	116,472	(6,144)	190,124

Treasurers Report 2002

The Association had a deficit of £4,097 during the year ended 31 December 2002 and has no material commitments or guarantees which could affect its future solvency. Major contributions to the reported deficit were a council decision to write off £2,369 stocks of "crystal books" for educational use and a reduction this year of £3,176 in the value of investments, down to £91,209 but still producing a healthy £6,097 of income. With total incoming resources of £118,519 and operating expenses of £116,472 we maintain a positive cash flow.

Council members have conducted a review of the reserves that the Association requires for sustaining its objectives. The major considerations are with regard to the long term funding of meetings, Bursaries and funding projected deficits from reduced investment income. Existing investments of £91,209 are considered adequate to meet these needs. A review of the major risks to which the Association is exposed has been conducted. The only consideration is with regard to its investments and to mitigate those risks the Association has all its

investments placed with an independent professional management company.

The £25,000 transferred to the IUCr congress for bursaries at the Geneva meeting in August 2002 has not yet been repaid. The Biological Structures Group closed a Building Society Account and took out an account with the Charities Aid Foundation paying better interest. The Association entered into an agreement with Taylor & Francis to publish highlights of the Spring Meeting proceedings in "Crystallography Reviews" and purchase copies for distribution to every member.

Sixteen Arnold Beevers Bursaries were awarded this year and the £4,000 awarded is up on last year. The schools crystal growing competition received sponsorship of £500. The Nottingham Spring Meeting awarded bursary funding of £5,400 to benefit 30 students with 17 being commercially sponsored. The Spring Meeting made a surplus of £7,154.

Crystallography News made a deficit of $\pounds1,356$ this year on a turnover of $\pounds28,587$. Production costs rose by

almost £9,000 to cover an increase in the number of informative pages. This quality publication has been well received by advertisers and is a major source of value to our membership. The BCA owes a debt of gratitude to its advertisers and sponsors who generously support our activities.

Subscriptions to International bodies (IUCr & ECA) have increased by $\pounds 1,567$ to reflect the full impact of the first full year of the 51% BCA and 49% Royal Society share of the IUCr subscription. Administration costs are a little higher this year at $\pounds 19,379$, up by $\pounds 1,289$ mainly due to an increase in travel expenditure in support of an extra planning meeting.

Membership income is up by £1,640 with eleven organisations paying Corporate Membership dues in 2002. Donations totalling £2,240 were received, up from £1,206 last year. Many of our members have signed Gift Aid declarations and a refund of £708 from the Inland Revenue further boosted the Arnold Beevers Bursary Fund.

The full BCA accounts for 2002 are available on request as an E-mail attached PDF file from the BCA admin office.



BCA Spring Meeting

BSG AGM

Biological Structures Group Sessions at BCA Spring Meeting

This year the Spring meeting was reorganised into a condensed format, to keep delegate costs down and to take up less of the Easter holiday. Another new feature this year was one day registration. A number of biological structure group delegates took advantage of the fact that BSG sessions were centred around the Wednesday when the BSG AGM was held. The lectures were all very well received. In addition to describing how high-throughput strategies have been implemented by groups in the UK and abroad, there were useful lessons to take home to a protein crystallography lab working on a more traditional hypothesis-first basis. These included experiences with protein expression, some extremely impressive robotics, enough about the usefulness and design of databases to encourage me to go home and start archiving my own group's experiments electronically, and the latest phasing methods. Speakers' travelling expenses this year were sponsored in part by TTP LabTech Ltd, whose robot which uses disposable needles was described in a talk by Marek Brzozowski.

York Exhibition Centre proved to be an excellent venue, both for the lectures and for the exhibition and posters which were combined in the intervening hall with a view over the lake. The compact spatial arrangement led to many lively discussions not only at Poster sessions but whenever there was a gap in the hectic schedule. This year, the David Blow Poster Prize was awarded to Jim Pflugrath et al. (Rigaku/MSC) for an excellent poster describing the use of a Chromium Anode on the home source to increase the size of the anomalous signal for sulphur (f"=1.14 e⁻ for CrK, f"=0.56 e⁻ for $CuK\alpha$ The resulting singlewavelength anomalous dispersion data was used to provide phasing for three structures: trypsin (24 kDa), thaumatin (22 kDa) and glucose isomerase (40 kDa).



Jim Plugrath receiving the David Blow Poster Prize; a large piece of Blue John mounted on a plinth (remuneration sponsored by TTP LabTech Ltd)

The runners-up were Echalier *et al.* (Warwick/Oxford) for a poster on using automated birefringence detection to find and assess crystallisation conditions and Miguel Ortiz-Lombardia *et al.* (Institut Pasteur, France) for a poster describing the crystal structure of the catalytic domain of PKNB, a serine/threonine kinase from Mycobacterium Tuberculosis.



Second prize was a copy of the book "Crystals and Life,a Personal Journey" by Cele Abad-Zapatero, which was kindly donated by Molecular Dimensions Ltd. The Max Perutz Memorial Lecture was introduced by David Blow who gave some fascinating background on the life and achievements of Max Perutz. The lecture itself was given by Venki Ramakrishnan. It was fitting that he comes from the Laboratory of Molecular Biophysics at Cambridge, where he determined the high resolution structure of the 30S ribosome. He gave an excellent overview of the history of ribosome structural biology as well as describing the insights from his high resolution structures.



Biological Structure Group AGM.

This was held on Wednesday 16th March after the morning sessions. Two items from the minutes should be noted in particular: It was proposed that the AGM should be held at the BSG Winter meeting in future. This was because more BSG members are generally present at the Winter meeting and also because time is extremely tight

BSG AGM

at the Spring meeting,

June 2003

particularly with the new format. This motion was accepted by the meeting so the next AGM will take place at the Winter meeting in London, 2003. Financially the BSG remains healthy, whilst it is walking a fine line between profit and loss each year for its two meetings. It was therefore agreed that the BSG should transfer bank interest accrued each year to the Arnold Beevers Memorial Bursary fund administered by the BCA, to be earmarked for spending on BSG members if possible. Elections were also held for the retiring officers: Chairman, Vice Chairman and Secretary/Treasurer and the retiring committee members: Andrew Leslie and Martin Noble. In the absence of other volunteers the Chairman and Secretary/Treasurer were persuaded to stand for a second term. Sheila Gover and Peter Moody were proposed as committee members. All were elected unopposed. The vicechairman's position, which has in the past been a 'grooming' post for a future chairman, is currently vacant. Nominations will be sought for the next AGM which will be held in December. The current committee is therefore composed as follows:

Chairman

Dr. Richard Pauptit (2003-2006)

Vice-Chairman Vacant

Secretary/Treasurer Dr. Andrea Hadfield (2003-2006)

Committee

Dr. Nick Keep (2001-2004) Dr. Harry Powell (2001-2004) Dr. Jon Cooper (2001-2004) Dr. Katy Brown (2001-2004)



Dr. Vilmos Fulop (2001-2004) Dr. Peter Moody (2003-2006) Dr. Sheila Gover (2003-2006) Biological Structure Group Committee, current and retiring members

Biological Structures Group Winter Meeting 2003

The BSG winter meeting will be held in London this year in December, on a topic to be finalised. Details will follow.

CCP4 inYork, January 2003 – Experimental Phasing.

The CCP4 meeting has a history of teaching those new to crystallography while at the sane time presenting recent advances and providing a relaxed and small forum for specialists to come together and share ideas. In the teaching tradition, each session at this year's meeting started with a talk giving an overview of the topic of the session. Garry Taylor and Randy Read started by introducing the phase problem, giving a rapid tour through the current methods of solving it; Elspeth Garman gave a vibrant talk on heavy atom preparation; Ana Gonzalez rated data collection

methods and introduced a "Michelin Star Guide" to synchrotrons; Ralf Grosse-Kunstleve described the different methods for finding heavy atom sites with a special emphasis on the challenges of symmetry and special positions; Simon Parsons explained twinning with the humble London Brick; and Gerard Bricogne presented impressive results from the new improved version of the popular phasing program "sharp". A recurring theme of the talks was radiation damage.

For some it was problem to be avoided, for others a tool to be exploited, Raimond Ravelli and Domenika Borek in particular presenting the case for the latter. The twinning session gave inspiration to those struggling with twinned data, as Zbignew Dauter, Anke Terwisscha van Scheltinga and Dimitriy Alexeev showing that twinned structures can be solved by MIR or MAD methods. The future of experimental phasing may have been predicted by Andy Stewart who described the experimental set-up for three beam interference studies at Cornell. The meeting seemed to be enjoyed at many levels, helped by the traditional degree of liquid refreshment.

Airlie McCoy

Dorothy Hodgkin Memorial

June 2003

The Founding of the Dorothy Hodgkin Memorial lecture

This Memorial lecture now forms part of the Oxford International Festival for Women held annually in March. In 1998 the Chair of the Festival, Anne Mobbs, felt that the UK's only woman Nobel Laureate in Chemistry deserved greater recognition, particularly in Oxford, where she did the work for which she gained a Nobel prize in 1964. Anne discussed it with Dorothy's old College, Somerville, the University Museum, where Dorothy had worked, and the Oxford AWiSE, (Association for Women in Science and Engineering, whose regular 'Oxford Science Lectures' began in December 1996; they thought one of the lectures in their Series could be designated as a 'Dorothy Hodgkin Memorial Lecture'.

A note about the launch of an appeal to fund a possible memorial for Dorothy in Oxford was published in the March 1998 issue of 'Crystallography News' (page 17). The appeal was launched at a meeting held in the University Museum on 19 March 1998 with the title 'An evening dedicated to the memory and achievements of The Amazing Dorothy Hodgkin'. I did not attend myself, but I was told that Georgina Ferry, Dorothy's biographer, interviewed Judith Howard, one of Dorothy's students, and encouraged her reminiscences about Dorothy's life. The June 1998 issue of 'Crystallography News' carried an Appeal flyer printed by the Oxford International Women's Week Collective, which gave a brief history of Dorothy's life of Science in Oxford and appealed for

donations for 2 possible projects, to commission a statue of Dorothy to be placed in the University Museum of Natural History and to finance childcare bursaries for Oxford women students.

Members of the BCA were asked to make donations and suggest a suitable memorial. All the comments I received thought that Dorothy would have hated a statue of herself, and the Childcare bursaries were a much better idea. Does anyone know whether the Chidcare Bursaries were ever funded?

This lecture is now sponsored jointly by the Oxford International Festival for Women, AWiSE (Association of Women in Science and Engineering), Somerville College who select the speaker and finance a reception afterwards and the Oxford University Museum of Natural History who donate the lecture room and reception facilities in the Museum.

Lectures in this series so far:

- 1. 4 Mar 1999 Professor Louise Johnson,
- "Dorothy Hodgkin and penicillin; 50 years from structure to present day understanding of Biosynthesis and bacterial resistance."
- 2. 13 Mar 2000 Professor Judith Howard,
- "The Interface of Chemistry and Biology Increasingly in Focus"
- 3. 15 May 2001 Professor Jenny Glusker "Vitamin B12 and Dorothy: Their impact on structural science"

 5 Mar 2002 Professor Pauline Harrison, "From Crystallography to Metals, Metabolism and Medicine"

Note: a set of links to web sites associated with this article, including a list of the 'Oxford Science lectures held so far' with reports of some of them, and websites of the sponsors can be found on the BCA website at http://bca.cryst.bbk.ac.uk/BCA/CNe ws/2003/Jun03/DHmem.htm

Dorothy Hodgkin's achievements recognised by others.

The British Crystallographic Association offers a triennial 'Dorothy Hodgkin prize', the first prize and associated lecture were given on her 80th birthday in 1991. (Details are on the BCA website http://bca.cryst.bbk.ac.uk/BCA/admi n/PRZ.html).

In May 1995 The Royal Society initiated a postdoctoral fellowship scheme known as 'the Dorothy Hodgkin Fellowships', these are intended primarily for parents of young children who need a high level of support and flexible working arrangements if they are not to abandon a scientific research career.

On 14 May 2001 the Royal Society of Chemistry presented a 'Chemistry Landmark' plaque with an accompanying ceremony in the University Museum, including a lecture given by Professor Sir Tom Blundell, a student of Dorothy's, on "Structural Biology and Crystallography Today: the influence of Dorothy Hodgkin on

current developments." The plaque is now fixed to the wall on the side of the archway of the main entrance to the Inorganic Chemistry Laboratory building in South Parks Road, Oxford. Jenny Glusker's Dorothy Hodgkin memorial lecture was given on the next day, 15 May 2001, as part of these celebrations.

Please send news of any other 'Dorothy Hodgkin' memorials to me, preferably by email to BCA@ISISE.RL.AC.UK so that I can maintain information about them on the BCA website.

Kate Crennell

The 5th Dorothy Hodgkin memorial lecture

"Pathogenic Proteins : how bacterial agents cause disease" presented by Dr. Claire Naylor, Birbeck College, University of London in the University Museum, Oxford at 5pm on 4 March 2003. Claire Naylor was a student at Somerville, gaining a 1st class degree in Chemistry in 1993 and a D.Phil in Crystallography in 1996. She is now a Royal Society Dorothy Hodgkin Fellow in the Protein Toxins Structure Group at Birkbeck College. She started by explaining that as all the previous lecturers in this series had been Dorothy's students, she felt more like one of Dorothy's grandchildren since her supervisor had been one of Dorothy's students. Her current research is on pathogenic proteins, particularly those secreted by bacteria, 99.9% of which are completely harmless to humans, and survive for years in their environment, but others are

toxic, for example, the streptococcus which causes sore throats, in other forms is the MRSA 'Super bug' resistant to most antibiotics. Her current interest is in lethal bacterial toxins including the Clostridium perfringens alphatoxin, and others associated with this one. This protein is widely distributed being found in human and animal gut and in the soil. One toxin is an entero toxin, a common cause of food poisoning which causes vomiting and diarrhea, but lasts only 48 hours in healthy adults and is rarely toxic. Epsilon toxin causes a nervous disorder in sheep, with a swelling of the brain which proves fatal in 48 hours. Beta toxin is common amongst people who have been existing on a meagre diet and then have a huge meal of more nourishing food. It forms a type of gangrene in the intestines. It was first detected in the victims from concentration camps, but now there is a vaccination against it.

The alpha toxin is associated with the disease 'gas-gangrene' which has been known for a long time. Graphic illustrations were shown of the unpleasant symptoms of gas gangrene. King Richard I is thought to have died from it, when his wound from a crossbow became infected. It has caused sudden death in Belgian bee colonies, 100,000 soldiers died from it during World War I and it caused an epidemic following a tidal wave in 1998 in Papua New Guinea. It is the first major toxin to be shown to be an enzyme, but the exact mechanism of how it destroys other cells is not known. It thrives in wounds where the supply of oxygen is limited. The only known cure is amputation of the affected limb.

Their research group is using several techniques to study the effects of the toxin on mammalian cells taken from the heart and lungs of cows. The alpha toxins surround healthy cells and destroy the protective cell surface membranes. These are made of phosphor lipid bilayers which are attacked by the toxin; it 'slices' off the hydrophilic head groups, leaving the hydrophobic tails within the cell, where they may trigger inflammation and release of calcium ions, which are used in signal transmission with neighbouring cells. The toxin has been crystallised and its structure found so that the conformation of the 'active site' which causes the damage can be studied in the hope of eventually developing a less drastic treatment than amputation for wounds infected with 'gas gangrene'. An additional problem is that these alpha toxins suppress the immune response but it is not known how they do this, so further studies are needed.

Margaret Adams thanked the lecturer for giving us this fascinating and well illustrated lecture despite suffering from a sore throat. We then adjourned for a reception in the mainhall of the University Museum with its Victorian architecture and dinosaur skeletons.

Kate Crennell

Education SIG

June 2003

Spring Meeting: Education SIG

The Education SIG at the BCA Annual meeting in 2003 held in York consisted of 3 parts: A summary of the replies received to the Survey of Undergraduate Crystallographic Teaching (Kate Crennell) Using 'cut out' models with young children to help them understand the principles of symmetry (Kate Crennell) Short courses for UK post graduate students (Bill Clegg, Chick Wilson, John Helliwell)

Replies to the Survey

No further replies were received following the report on page 8 of the September 2002 issue of 'Crystallography News'. The paper survey had appeared in 2 issues of our newsletter, it had been sent out with the Mineralogical Society Bulletin and distributed to delegates to the International Mineralogical Association meeting in Edinburgh in September. The Institute of Materials had kindly distributed it to the Heads of Materials Departments in the UK by email.

The 22 replies came from Departments of Chemistry (8), Materials and Engineering (5), Biochemistry(4), Physics (3), Crystallography (1) and one enthusiast who sent in both a paper and an electronic version by email. Several physicist members mentioned during the meeting that they had not returned the survey because crystallography is no longer taught to physics undergraduates in their University. Is this a worrying trend which the BCA should try to counteract? We did receive some useful suggestions as to how the BCA might help lecturers, these are listed on the website

http://bca.cryst.bbk.ac.uk/BCA/ed/su rvey/result/htm

One problem mentioned by several people was the difficulties some students have in understanding symmetry operations and point groups, another sent in a set of their practical exercises which I hope to convert for use on the website.

Using Crystal Shapes with school children

Rockwatch is the name of a series of Saturday morning meetings for school children interested in geology. On 8 February 2003 they met in the Information Centre of Crystal Palace Park when the subject was 'Crystals, an aid to mineral identification'.

The meeting was very well attended, over 20 children and some parents came to learn a little about crystal shapes, try their hand at the guiz, (some guestions are given below) and try making up their own crystal shapes using the newly devised set of crystal classes 'cut out models' which I made for these people and which can now be downloaded from the BCA website and used for any students. The organiser, Austin Lockwood, of the Ravensbourne Geological Society kindly sent me some photographs of the children busy making up their own crystals,



He also sent an example leaflet showing the type of information they give out at each session, and the quiz for this particular session. The students insist they must have a quiz and enjoy doing them. Some sample questions are given below to show the sort of questions which the children enjoy. The workshop is to be repeated at High Elms Country Park in Kent on Saturday 23 August 2003. I shall be on holiday then, but if there is anyone who would be interested in watching with a view to running a similar workshop in their area I am sure they would be welcome. Contact Austin Lockwood either by phone tel: 020 8650 5566 or email

austin.lockwood@btopenworld.com

Some typical quiz questions:

- What is the name of the instrument used to measure the angles of crystals?
 1.Clinometer,
 2.Thermometer
 3 Goniometer
- 2. Where are 'perfect' crystals to be found?1. In Cornwall2. In museums
 - 3. In models
- 3. What is the state of solid disorder called?1.Amorphous2. Amorous3. My bedroom

- 4. Which of these minerals does not crystallize in a cubic form?
 - 1. Calcite
 - 2. Galena
 - 3. Pyrite

The new set of 'crystal class cut out models' can be downloaded from the BCA education web page models.htm. There are 8 models, one for each class and an extra one as a puzzle. In addition to the planar net which can be constructed to make the model there are several 3D views of the model. Students are asked to identify the symmetry axis along which the model is viewed and write the appropriate symmetry symbol on the model itself. Although first used with children, these models should also help undergraduates understand the different types of symmetry. Why not try them on your students? Then send me your comments, I do not teach myself, so lack experience of students' difficulties.

Short Crystallographic Courses for UK students

These are mostly short courses lasting between one or two weeks on particular topics of interest to graduates just starting research for their Ph.D. They are run annually or biennially. Although intended for British students, students from elsewhere may be enrolled if there is spare capacity; the courses have proved popular with overseas students whose command of spoken English is good enough for such intensive courses. Other courses are run by large scientific establishments, usually based on particle accelerators, intended to show potential users of the

facilities the experimental techniques using the radiation produced from the accelerator, either synchrotron radiation or neutrons.

There are occasional other one-off short courses on single topics, such as that to be run by the University of Sheffield from June 17th to 20th 2003 'A Practical Introduction to Chemoinformatics'. This has particular emphasis on applications in modern drug discovery. Like the other courses it is a mixture of hands-on workshops, lectures and informal discussions. A key focus is on the underlying theory rather than just teaching which buttons to press on a particular piece of software. Sometime these courses grow into year long M.Sc courses such as that on bioinformatics run by the University of York. I am setting up a new web page listing the short courses of interest to crystallographers which do not lead to a formal academic qualification. Please send me news of your courses. This page will be linked to the BCA education web pages at

http://bca.cryst.bbk.ac.uk/BCA/ed/co urses.htm

BCA ORGANISED COURSES - the CCG 'Summer' School

Members of the Chemical Crystallography Group of the BCA run an 'Intensive Course in X-Ray Structural Analysis' lasting about a week every other year. The first one was held in Aston University in 1985, organised by Judith Howard who was then at Bristol and David Watkin of Oxford; the most recent was in Durham the week before the BCA Annual meeting in 2003. The next one will be in 2005, details of which will be placed on the CCG pages of the BCA website, when the exact dates are known. As well as lectures, there are less formal occasions, when students are encouraged to ask about topics which their previous education has not covered, allowing tutors to provide special lectures for a few students. Increasingly tutors find that chemistry students learn less mathematics these days; for example, in 2003 some had not previously met vectors or matrices and special tuition was arranged for them.

BCA ORGANISED COURSES - the BSG 'Summer' School

Encouraged by the success of the CCG Course, members of the Biological Structures Group, Margaret Adams and Hilary Muirhead, organised a 'Graduate Summer School in Protein Crystallography' in July 1990. This followed the same pattern as the CCG course initially; it ran every other year and was a great success. More recently at the request of the Research Councils, and with sponsorship from them, the school runs every year, one year in Bristol and the next in St.Andrews, Scotland, usually in September. This year it is to be held from 9 to 16 September 2003 in St.Andrews, details from their website.

PCG AGM

June 2003

AGM of the PCG

27 members of the group attended the 60th Annual General Meeting of the PCG at York. Six members of the PCG Committee were present, including Pam Thomas (Chair) and John Evans (Hon. Sec./Treasurer). It was reported that the 2002-2003 year had been a busy and successful one for the PCG. The autumn meeting was

organised by Dave Allan/Pam Thomas and was held on December 11th 2002 in Edinburgh. The meeting was well attended and was scientifically excellent. ISIS/PCG co-sponsored a workshop on Magnetic Rietveld refinement held at Cosener's house on 12/13th December 2002. All both of these PCG activities have already appeared in earlier issues of Crystallography News. At the York BCA, PCG were responsible for three sessions on each of **High Energy Diffraction** (organized by Steve Collins), on Structure Determination from Powders (organized by John Evans) and on Crystallography for Technology (organized by Pam Thomas) and reports of these sessions appear in the current issue. Just prior to the BCA meeting, PCG provided a session on charge/orbital ordering, organized by Paolo Radaelli, at the CMMP meeting in Belfast. Both the talks and the ensuing discussions were of a high standard. General attendance at the whole CMMP meeting was low, something that is being looked into by the IOP

> division. In this context, it was noted that the future frequency of major CMMP meetings may become biannual to reflect the trend away from large generalized conferences to smaller more specialized meetings. During discussion of future activities of the PCG,

it was agreed that training/tutorial sessions are an important role of the group, and should be emphasised. Suggestions for workshops on Rietveld refinement, diffraction methods (such as reflectometry), symmetry and diffuse scattering were made and it was requested that PCG officially lobby the IOP about the inclusion of crystallography-related material in future school and university Physics syllabi. It was noted that the financial position of the PCG is healthy. With this in mind, PCG members were reminded that they could put in requests for travel support to relevant national and international meetings. Pam Thomas was reelected as the PCG representative to the CMMP and two new ordinary members of the PCG Committee were elected unopposed: Thomas Lyford of PanAlytical Ltd and John Loveday of Edinburgh University.



The winner of the PCG poster prize is Clivia Hejny for "Complex Structural Behaviour of High Pressure of Selenium and Tellurium" by C.Hejny, M.I.McMahon and R.J.Nelmes at the School of Physics and Centre for Science at Extreme Conditions, Edinburgh.



Back row, left to right: Jonathon Wasse (UCL), Jeremy Cockroft (Birkbeck), John Evans (Durham, Secretary), John Loveday (Edinburgh). Front row, left to right: Steve Collins (Diamond), Dave Allan (Edinburgh), Pam Thomas (Warwick, Chairman), Tom Lyford (PANalytical Ltd), Paolo Radaelli (R.A.L., ViceChairman).

places were taken within 24 hours of the course announcement. The meeting was organised by Paolo Radaelli with teaching from Andrew Wills and Juan Rodriguez-Carvajal as well as Paolo himself. Reports on

BCA Spring Meeting

Spring Meeting: Crystallography and Technology

The Crystallography and Technology Session, organized by the PCG, comprised five invited talks united by the theme of the application of x-ray or neutron diffraction/scattering methods to technologically-important or physically-interesting materials. Dr Tom Hase from Durham began the morning session (at the anti-social hour of 8.30 a.m., the morning after the Conference Dinner) with a clear account of his studies of colossal and giant magnetoresistive materials (CMR and GMR, respectively). GMR materials are magnetic multiplayer systems whereas CMR systems, such as the double-perovskite La_{1-x}Sr_xMnO₃ are bulk materials, in which the Mn³⁺/Mn⁴⁺ ordering is key to the CMR effect. To understand GMR systems and improve their functionality, study of interface roughness, grain boundary effects and domain walls are important whereas in CMR materials, in-plane correlations are important. Tom described a variety of x-ray scattering experiments, principally using synchrotron sources, designed to examine interface roughness and in-plane correlations with line-width analysis being employed to extract physical parameters.

The following talk, by Dr. Petra Rejmankova-Pernot from the ESRF, gave a thorough explanation of xray imaging experiments aimed at examining the detailed atomiclevel structure of ferroelectric domains walls in periodically-poled nonlinear optical crystals. She explained why these frequencyconversion devices are important and how these structures, which have periods on the scale of 10's of microns, can be studied using the exceptionally high lateral coherence of the beam at Station ID19 of the ESRF to see the periodic domains as a periodic phase grating. The importance of freespace propagation of coherent diffracted beams of the sample to give interference images of Fresnel type was emphasized and the methodology by which phase information could be gathered from the domain wall regions was explained. Finally, Petra showed how this novel technique had been effectively applied to obtain new information about the atomic-level structure of domain walls in crystals of the KTiOPO₄ (KTP) family.

In a return to magnetic systems, Professor Steve Lee from St Andrews turned to neutron small angle scattering to elucidate information about magnetic nanoparticles in magnetic recording media. The nanoparticles have a cobalt-rich ferromagnetic core and chromiumrich non-magnetic shell. The question Steve is trying to answer using scattering techniques, is how the magnetic moments are aligned when the nano-particles are assembled together. Steve explained the methodology employed to extract the small magnetic scattering signal from the large overall small-angle scattering signal and explained the difficulty in extracting the true magnetic structure, as opposed to an average magnetic structure, from the data. He showed a preliminary model for the arrangement (effectively, a magnetic crystal structure) of the nano-particles with an average

magnetic grain size of 110 Å.

After the coffee break, the session continued with a very clear exposition of the principles and practice of characterizing semiconductor thin films by Dr. Tricia Kidd from PanAlytical. She concentrated on her studies of a vertical-cavity surface-emitting laser (VCSEL) multi-layer structure using high-resolution x-ray diffraction in a home laboratory rather than at a central facility. Her task was to elucidate for the device growers whether they had made the device that they expected. This presented a challenge since it is a complex device, with AlGaAs multilayers sandwiching an active $In_xGa_{[1-x]}P$ quantum well all on a GaAs substrate. Tricia guided us through the experimental methodology employed e.g., the choice of x-ray optics, type of scans and choice of reflections, before discussing the method of data fitting, which she confined to the assumption of entirely perfect crystals treated using the dynamical theory. Whereas she was satisfied that she was able to answer the device-growers questions to within the tolerance of their certainty in growing, she discussed the possibility of pushing the x-ray analysis further by possibly taking the structural crystallographer's approach, measuring multireflection data and conducting a multi-parameter refinement. At the moment, this remained a task for the future.

The session was ably brought to a close by final-year PhD student Simon Levett from Warwick, who was standing in for his supervisor Professor Don Paul. The period of the vortex lattice is of order 1000 Å

BCA Spring Meeting

June 2003

so, once more, small-angle neutron scattering was the technique of choice for the study. For industrial applications, it is necessary to fix the vortex lattice to avoid dissipation of energy in the superconductor and, therefore, it is necessary to have a fundamental understanding of how the lattice behaves. Simon described the careful experiments to elucidate the vortex lattice and to monitor its behaviour as a function of temperature and magnetic field and the theory of the formation of square and hexagonal lattice arrangements in different superconductor systems. He showed a first-order phase transition between different orientations of the square lattice in TmNi₂B₂C, which sparked analogies with other types of "structural" phase transitions. Simon introduced members of the audience to the idea of a "Bragg glass", which seems to be a material with long-range order that changes (through a creep process) over time. The mention of Bragg's name brought the crystallographers in the audience alive and some discussion ensued as to whether a "Bragg glass" was just a disordered crystal by another name. However, it was decided that the creep aspect made it distinct - further comments on a postcard please.

In all, the session showed an impressive range of neutron and xray scattering experiments being conducted on physically-interesting samples of every type to elucidate "structure" (in its broadest sense) in a range of length scales of four orders of magnitude. Structural condensed matter physics is evidently alive and well! Spring Meeting: Structure Solution from Powders: CCG-PCG

The final lectures of the Spring meeting took place in a joint CCG-PCG session on "Structure Solution from Powders" cochaired by Paul Raithby and John Evans. Attendees were treated to 5 excellent lectures on different aspects of structure solution/refinement from powder diffraction data, giving a high quality end to the York Meeting.

Yuri Andreev (St Andrews) started the session off with a wonderful overview of the huge advances made in determining the structure and properties of polymer electrolytes from powder diffraction data materials of immense potential technological importance for which it is often impossible to obtain single crystals. Louise Male showed the complexity of problems that can now be tackled by giving examples of some organometallic species that have been studied at Bath. Harriott Nowell (Cambridge) addressed a different aspect of the problem of structure determination from powders how to treat the restraints that are often required during the Rietveld refinement stage of powder work. The methodology she presented, based on knowledge contained in the Cambridge Structural Database, seems likely to be of importance as these methods develop.

The last two talks of the afternoon were given by MaryJane Tremayne of

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Birmingham and Alastair Florence of Strathclyde. MaryJane presented work on a new Differential Evolution algorithm for structure solution which offers potential advances in terms of the complexity of structures it can tackle and the computational time required to solve a particular problem. Alastair showed how low temperature studies of powdered samples in the lab are of importance not only in improving data quality via the reduction of atomic motion, but also due to the fact that anisotropic thermal expansion can lead to different patterns of peak overlap at different temperatures, thus potentially increasing the information content of a powder diffraction pattern.

The series of excellent talks presented shows that this is an exciting and rapidly developing area of crystallography.



Pam Thomas

The PANalytical Prize Lecture by John Loveday

The winner of the 2003 PANalytical Prize for Physical Crystallography is Dr. John Loveday from Edinburgh University. John received his prize for his high-pressure studies of gas hydrates and clathrate hydrates, the results of which have implications for the understanding of Neptune, Uranus and Titan, the largest moon of Saturn. In his excellent prize-winning lecture at the BCA meeting in York, John chose to concentrate on the use of his studies for modelling the atmosphere of Titan, thereby illustrating the importance of high-pressure studies on this planet for understanding the Universe beyond. In the history of the PANalytical (formerly Philips) prize, I cannot remember a more "far-reaching" (in the sense of distance, at least) application of Physical Crystallography than this one, although readers of Crystallography News may beg to differ with me. The lecture, a written version of which follows in the September edition, was welldelivered and of high scientific quality demonstrating that once again, the PanAlytical prize has been very worthily awarded. Congratulations again to John Loveday.

Pam Thomas



Diamond Light Source Ground breaking ceremony, Rutherford Appleton Laboratory , 12 March 2003

The organisers wisely imported a Marguee to shelter the visitors and officials of diamond from the worst of the weather, which can be wet and very windy in March on the flat site which was formerly the RAL football pitch. Inside the Marquee over 150 quests had a welcome coffee and a chance to see the exhibition of plans for the synchrotron itself, the first beamlines, to admire the latest model of the site and to mingle with the diamond staff. The guests included local residents and Council officials as well as potential diamond users.



Colin Norris (Leicester University), Interim Science Director (Physical Sciences) of the diamond Scientific Advisory Committee, deep in discussion with a BCA Honorary member, Andrew Lang (Bristol University),



BCA Secretary, Christine Cardin, talks with local residents well known local water colour artist, Ken Messer and his wife Dilys)

We then walked to the nearby Lecture Theatre for short presentations, starting with the Chief Executive of the Diamond Light Source, Prof Gerhard Materlik who reminded us that diamond is currently financed 86% by the CCLRC and 14% by the Wellcome Trust. In the year since the formation of the company to construct and run diamond, the key people have been recruited, there are now 50 employees and they hope for twice that by the end of the year. Enabling work on the site has begun, installation of the accelerator should begin in September 2004, the office block is scheduled for completion in November 2004, the first beam in the storage ring by 2006 and the first users in 2006/7.

Prof John Wood. Chief Executive of the CCLRC, welcomed us with a description of the laboratories managed by the CCLRC enabling UK Scientists to do World Class Science. International collaborations are being encouraged, especially with other European countries. Dr John Taylor, Director General of the Research Councils, spoke on the impact of diamond on UK Science. He reminded us that it had been first proposed by the Woolfson report of 1993 and he was very glad to be here today to see construction begin, on this the largest UK Science project for the last 30 years. Dr Michael Morgan, Consultant on special projects for the Wellcome Trust, explained how the new synchrotron was essential to the realisation of the medical potential of gene sequencing. He had formerly worked on the Wellcome funded Sanger Centre in Cambridge. They are considering setting up a 'Structural Genomics Consortium' in collaboration with Canada, with a UK site probably near to diamond. Other projects may be a 'UK

Ground Breaking

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Biobank' and 'Clinical Research facilities' where they will encourage doctors to put the patient first. Prof Phil Withers began his talk 'For now we see through a glass darkly' by pointing out how little is known about the materials used in transport today. Did those of us who came by plane realise that ageing aircraft can have as many as 100,000 rivet holes, at least 5% of which are cracked? He also discussed ways of measuring stress in railway lines, in human joints and how to watch the internal changes which occur as composite fibres break. He emphasised the need to remain flexible because we cannot know today what instrumentation we will need in 20 years time for the important future experiments of tomorrow.

All the speakers moved to the front for the 'Question and Answer' session, including the following questions and answers:

- We have heard that the facility will evolve in time. How is its direction decided? By consultation with the User Community, they will continue with a Science Advisory committee to set the priorities amongst the competing science areas wanting new beamlines or instrumentation.
- Is this work likely to have an impact of the fusion research taking place at nearby Culham? Yes, there is already dialogue between the fusion scientists and the materials scientists who will be using diamond.
- 3. What are the main challenges in this project?
- a) Construction, the machine base must be mechanically stable to small tolerances in all weathers while mounted on chalk bed rock.

- b) Machine operation must be stable over long time periods.
- c) Beam lines, how do we design the best beam lines for future experiments which we do not yet know we want to do.
- 4. Will there be opportunities for local high-tech industries to participate in this project? Yes, diamond is working towards a 'campus model' of collaboration, but the local industries have to be encouraged to participate. A report should be published within a few weeks detailing likely 'spin-off' and opportunities for local industries.
- 5. What is diamond's commitment to education in the locality? They will encourage their scientists to visit local schools to talk enthusiastically about their work. They plan to work with local Universities to form a local centre for Excellence in Science teaching in the schools. They also plan to have vocational training and apprenticeship schemes in collaboration with local colleges of further education.
- 6. Is the diamond organisation satisfied that the local infrastructure in this area has enough facilities for a project of this scale? They are building a new access road to the diamond site. They realise that house prices in the area are very high. However, they are talking to the regional development authority who they hope will develop suitable support facilities.

The questioner was urged to discuss his problems with local councillors and MPs in the audience over the buffet lunch.





We then returned to the marguee for the Ground Breaking ceremony where Dr. John Taylor did a neat job of turf cutting with an environmentally friendly spade, followed by the incredibly clean and sparkling yellow mechanical digger cutting another ceremonial sod, this one rather larger. Although the inscription on the spade showed that it was intended as a commemorative present to Dr Taylor, he felt it rightly belonged in a 'diamond museum' so gave it to Prof Materlik for safe keeping. A buffet lunch followed, where some crystallographers managed to find seats at a table. Others stood up in



Ground Breaking

Diamond Update



conversation with ISIS employees, showing that the inter-disciplinary contacts referred to by Dr Taylor were already taking place.

Kate Crennell

Diamond Update – Meeting of the Diamond Special Interest Group

The Diamond SIG met at 12 noon on Thursday, 17th April, during The BCA Spring Meeting at York. The session started with a short presentation from Dr Jeremy Karl Cockcroft (Birkbeck College, London), the coordinator of the proposal for the Diamond High **Resolution Powder Diffraction** Station. Jeremy indicated that since the beamline had been approved in the Summer of 2002 there had been few developments. The next major advance would be when a beamline scientist was appointed for this Station. However, there have been important developments at the Diamond Site. The ground breaking ceremony took place on the 11th March.

Next, Professor Paul Raithby (Bath), the coordinator of the bid for the Diamond Single Crystal X-ray Diffraction Station, reported that a full proposal, supported by 76 Expressions of Interest from 100 principal investigators, had been submitted before the deadline of the 12th March to the Diamond Scientific Advisory Committee (SAC). The next step is an oral submission at the Diamond Open Meeting at the Rutherford Appleton Laboratory on Tuesday, 20th May. Paul Raithby gave an overview of the submission, prepared with the help of the working group:

Professor Bill Clegg (Newcastle/Daresbury Laboratory) Dr Jacqui Cole (Cambridge) Professor Russell Morris (St Andrews) Dr Simon Teat (Daresbury Laboratory) Professor Chick Wilson (RAL) Dr Claire Wilson (Nottingham)

In the presentation he outlined six themes in structural science that could be developed and extended using a Diamond single crystal facility. These themes included:

- Underpinning the frontiers of science and technology
- Charge density, from electron density to molecular properties
- Excited state crystallography
- Anomalous dispersion studies enhanced detail at the edge
- Disorder and its relation to physical properties

• Structure under change Many planned experiments in these areas could not be undertaken on any existing synchrotron facility, and

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Paul emphasised the complementarity with experiments that could be carried out at other facilities worldwide.

This theme of complementarity with other techniques and facilities was elegantly developed in the final presentation entitled "New Exciting Science at Big Facilities", given by Professor Chick Wilson (RAL). Chick outlined some of the opportunities that are being made available to structural scientists by current and future developments at the Central Facilities. Chick described new instrumentation at ISIS and the ILL neutron facilities, and discussed the major initiatives of the Millenium Programme (ILL) and the Second Target Station (ISIS). He then extended the discussion to the complementary facilities including the Central Laser Facility at RAL and high performance computing facilities. Chick also emphasised that the Central Facilities were not just there in the form of equipment for the user community, but also ran science-enabling initiatives that were supporting and providing studentship in a number of key areas of science. Chick completed his talk with a few thoughts on the potential that Diamond has to drive exciting science forward over the coming decades.

Paul Raithby Co-ordinator, BCA Diamond SIG

Questions

Puzzle Corner

Questions Answered in 'The Times' in April 2003

A reader on the Times had asked for help in finding the next 2 lines to one of the variations of 'Twinkle, twinkle, little star' which he had heard 40 years ago and could no longer remember.

John Price of East Molesey, Surrey wrote:

This version was recited by my grandmother in the 1940s:

Scintillate, scintillate globule vivific Fain would I fathom thy nature specific Loftily poised in ether capacious Strongly resembling a gem carbonaceous.

What does BCA mean to you?

Occasionally I get emails complaining that the sender is looking for the British Cement Association, came upon our web site by mistake, and asked me where to find the 'BCA' site they really wanted. These thoughts are prompted by a kind member, Richard Bytheway, who sent me an email on 4th March about the old webpage of 'TLAs', (Three letter acronyms) with definitions of the ones I had been unable to find.

(http://bca.cryst.bbk.ac.uk/BCA/CNews/TLAS.html) He thoughtfully gave a Website

(http://www.acronymfinder.com/) with a list of definitions, so I looked for 'BCA' and found 36 abbreviations listed including 'Bombay Cricket Association', 'British Car Auctions' and ending with 'Business Case Analysis'. I offered an additional entry for the 'British Crystallographic Association'; the site owners like to check the credentials of all their entries, so perhaps by the time you read this there will be even more meanings of BCA!

Kate Crennell

Puzzle Corner

This month's puzzle is easy if you have access to International Tables, Volume E (see review in this issue)! Classify each of the following friezes to one of the 7 frieze groups:

ppppppp
 xxxxxxx
 pqpqpq
 pqbdpqbd
 cccccc
 pdpdpd
 pbpbpb

Answers, please, to the Editor before 25 July, 2003.

The solution to last month's cross-group is: Across: 2: P63/mmc; 3: P212121; 4:Pbca; 6: Cmce (Cmca); 10: Imma; 12: Ia-3d 13: Pcab; 14: I4/mmm. Down: 1: P21/c; 2: P21; 5: B2; 7: Cc; 8: Im; 9: R-3; 11: Aea2 (Aba2); 13: Pm. No one had a completely correct solution, but joint prizes to Jim Trotter of Vancouver and Alice Dawson of Edinburgh, neither of whom had any assistance from the Editor. Congratulations! Incidentally, in Alice's lab, that new-fangled e-glide is currently referred to as an "improper axis of evil".



Meetings of Interest

June 2003

Meetings of interest Further information may be obtained from the website given. 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, bob@gould.ca

1-5 June 2003

High Pressure Crystallography, Erice, Italy, [http://www.geomin.unibo.it/orgv/erice/ highpres.htm]

7-11 June 2003

The Clay Minerals Society 40th Annual Meeting jointly with the Mineralogical Society of America, Athens, Georgia, USA. [http://cms.lanl.gov]

9-13 June 2003

Advanced Methods in X-ray Powder Diffraction, ICDD clinic, Newtown Square PA, USA. [http://www.icdd.com]

15-20 June 2003

The 4th International Workshop on Physical Characterization of Pharmaceutical Solids, Danbury, CT USA [http://www.assainternational.com]

16-17 June 2003

Single-Crystal Diffuse Scattering at Pulsed Neutron Sources, Argonne National Laboratory, USA. [http://www.neutron.anl.gov/diffuse/]

17-25 June 2003

EMBO workshop on Strategies in in Macromolecular Structure Determination at 3rd Generation Synchrotron Sites, Grenoble, FRANCE, [http://www.esrf.fr/Conferences/EMBO2 003/Application/

19-20 June 2003

3rd generation sources: highlights and future perspectives. Workshop at the ESRF, in Grenoble, France [http://www.esrf.fr/Conferences/XAS/

19-22 June 2003

12th Croatian Slovenian Crystallographic Meeting , National Park, Plitvice Lakes, Croatia,

[http://www.chem.pmf.hr/~hkz/plitvice]

20-25 June 2003

LERM 2003, International Symposium on the Role of Light Elements in Rockforming Minerals, Nové Mestona, Czech Republic.

[http://sci.muni.cz/~lerm/index.htm/]

21-25 June 2003

5th EMU School: Ultra-high pressure metamorphism, Budapest, Hungary, [http://www.univie.ac.at/Mineralogie/E MU

22-25 June 2003

XIIth International Workshop on Quantum Atomic and Molecular Tunnelling in Solids, University of Florida in Gainesville, [http://www.clas.ufl.edu/QAMTS]

22-26 June 2003

Euroclay 2003, Modena, Italy [http://www.unimo.it/euroclay2003/]

22-27 June 2003.

The 12th International Conference on Xray Absorption Fine Structure (XAFS 12), Malmö, Sweden, [http://xafs12.maxlab.lu.se/]

22-27 June 2003

8th International Kimberlite Conference, Victoria, BC, Canada. [http://www.venuewest.com/]

22-27 June 2003

Gordon Research Conference on Thin Film and Crystal Growth Mechanisms, Mount Holyoke College, South Hadley, MA, USA.

[http://www.chem.cornell.edu/ThinFilm/]

27-30 June 2003

2nd Conference on Modelling Of Protein Interactions In Genomes, Stony Brook, NY,USA ⁻

29 June - 3 July 2003

11th Annual International Conference of Intelligent Systems for Molecular Biology, Brisbane, Australia [http://www.ismb.org/ismb2003]

30 June-4 July 2003

ICESS-9 - International Conference on Electronic Spectroscopy and Structure, Uppsala, Sweden, [http://www.fysik.uu.se/icess9/]

2-9 July 2003

Course on Synchrotron Radiation and Free-Electron Lasers, Brunnen, Switzerland. [http://cas.web.cern.ch/cas/welcomebrunnen2.html]

7–9 July 2003

Workshop on X-Ray Diffraction. IMRE -University of Havana, Cuba. [mailto:mhc@imre.oc.uh.cu]

7-10 juillet 2003

Le colloque de l'Association Francaise de Cristallographie , Caen, France [http://wwwcrismat.ismra.fr/afc2003/index.html/

8-11 July 2003

WIRMS 2003 - International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources, Lake Tahoe, CA, USA. [http://infrared.als.lbl.gov/WIRMS/]

9-10 July 2003

First Workshop of the International Consortium on Ultra-Small-Angle Scattering (IConUSAS), Oak Ridge, TN, USA

[http://www.sns.gov/iconusas_workshop/ iconusas_2003.htm]

14-17 July 2003

International Workshop on the Scientific Opportunities with Cold Neutron Timeof-Flight Spectroscopy, Washington DC, USA [http://sokol.phys.psu.edu/cnw/]

20-24 July 2003

The Fifteenth American Conference on Crystal Growth and Epitaxy (ACCGE-15). Keystone, CO, USA. [http://www.crystalgrowth.org/conferen ces/ACCGE15/index.html]

Meetings of Interest

June 2003

21-25 July 2003

5th European Mineralogical Union (EMU) school, Budapest, Hungary [http://www.univie.ac.at/Mineralogie/EMU]

24-26 July 2003

2003 Current Trends in Microcalorimetry, Boston Marriott Copley Plaza, Boston, MA, USA [http://www.microcalorimetry.com/semi nars/2003Conference2.html]

25-26 July 2003

IUBMB Satellite Meeting on Biomolecular Structure, Cellular Structure and Drug Discovery, University of Toronto, ON, Canada [http://phm.utoronto.ca/~iubmb/]

26-31 July 2003

American Crystallographic Association Annual Meeting, ACA 2003, Cincinnati, Ohio, USA, [http://www.hwi.buffalo.edu/ACA/ACA-Annual/futuremeetings.htm

29 July – 1 August 2003 Materials Chemistry, MC6: Frontiers and Interfaces, University of Sheffield. [http://www.rsc.org/lap/confs/mc6.htm/]

3-6 August 2003

Polarised Neutrons and Synchrotrons Xrays for Magnetism, Venice, Italy [http://venice.infm.it]

10-13 August 2003

Australian Crystallographic Association '03/Crystal-23, Cable Beach Club Resort, Broome, WA, Australia, [http://www.crystal.uwa.edu.au/Crystals DownUnder/]

10-23 August 2003

The fifth United States National School on Neutron and X-ray Scattering, Argonne National Laboratory, USA [http://www.dep.anl.gov/nx/

14-15 August 2003 Workshop on Biological Structure, Cable Beach Club Resort, Broome, WA,

Australia, [http://www.crystal.uwa.edu.au/Crystals DownUnder/]

14-19 August 2003

Sagamore Meeting (IUCr Commission on Charge, Spin and Momentum Densities), Cable Beach Club Resort, Broome, WA, Australia. [http://www.crystal.uwa.edu.au/Crystals DownUnder/]

16-22 August, 2003 Symmetry 2003, Budapest, Hungary [http://www.conferences.hu/symmetry2003/]

21-22 August 2003 African Neutron Diffraction Meeting, Pretoria, South Africa. [http://www.sacrs.org.za/andm/index.html]

22-23 August 2003

Workshop on X-ray Science with Coherent Radiation - satellite meeting of SRI2003, Berkeley, CA, USA. [http://www.chess.cornell.edu/Meetings/ index.html]

24th August 2003

Free One-day Single Crystal and Powder Diffraction Software Workshop With ECM21: Durban, South Africa [http://www.ccp14.ac.uk/projects/ecm21durban2003/]

24-30 August 2003

21st European Crystallographic Meeting, Durban, South Africa, [http://www.ecm21-africa.co.za/]

25-29 August 2003

Eighth International Conference on Synchrotron Radiation Instrumentation, San Francisco, CA, USA [http://www.sri2003.lbl.gov/]

1 - 4 September 2003 The XIX Conference on Applied Crystallography, Krakow, Poland [http://crystallography.us.edu.pl/]

2-6 September 2003

ECNS 2003 European Conference on Neutron Scattering, Montpellier, France, [http://www.sfn.asso.fr/]

3-6 September 2003

9th European Conference on Solid State Chemistry, Stuttgart, Germany [http://www.mpistuttgart.mpg.de/conf/ecssc9/]

3-7 September 2003

Fifth International Conference On Molecular Structural Biology, Vienna, Austria.

4-7 September 2003

Summer School on Polycrystalline Structure Determination by Direct Methods, Krakow, Poland [http://crystallography.us.edu.pl/]

7-12 September 2003

13th V.M. Goldschmidt Conference, Kurashiki, Japan [http://www.icsinc.co.jp/gold2003]

8-11 September 2003

Biocrystallography course: From gene to drug, Centre of Excellence in Biocrystallography of the University of Trieste, Italy.

8-13 September 2003 Aperiodic-2003, Belo Horizonte, Brazil, [http://www.fisica.ufmg.br/~ap2003/]

8-18 September 2003

8th Oxford School on Neutron Scattering, University of Oxford, Mansfield College [http://www.isis.rl.ac.uk/conferences/osns2003/]

12-14 September 2003

Materials Discussion 6: Controlled Polymer Architectures - from Micro to Meso Scale, Durham, UK [http://www.rsc.org/lap/confs/md6.htm]

14-19 September 2003

Structure Solution from Powder Diffraction Data, Stara Lesna, Slovak Republic. [http://www.sspd-03.sav.sk]

15-19 September 2003

XV International Conference on X-ray Diffraction and Crystal Chemistry of Minerals, St Petersburg State University, Russia [http://www.lcm3b.u-

nancy.fr/cims/forthcoming.htm#STPeterburg]

Meetings of Interest

June 2003

18-23 September 2003

SHELX Workshop, University of Göttingen, Germany [http://shelx.uniac.gwdg.de/SHELX/workshop.htm]

22-25 September 2003

DyProSo XXIX conference / Elettra (Dynamical Properties of Solids), Trieste, Italy. [http://www.elettra.trieste.it/dyproso]

22-26 September 2003

XVII International Congress on X-ray Optics and Microanalysis", Chamonix Mont Blanc, France [http://www.esrf.fr/Conferences/ICXOM]

6-10 October 2003

Introduction & Advanced X-Ray Diffraction For Pharmaceutical Applications, Danbury, CT, USA http://www.assainternational.com]

15-17 October 2003

Polymorph Screening - Techniques & Applications, Stamford, Connecticut, USA http://www.assainternational.com]

24 October 2003

36th SRC Users' Meeting, Stoughton, WI, USA, [http://www.src.wisc.edu/meetings/SRC_ UM2003/default.htm]

24-26 October 2003

Workshop on Radiation-based Analytical Techniques. Cape Town, South Africa. [http://www.medrad.tlabs.ac.za/isrp9.htm/]

27-30 October 2003

International Symposium on Pulsed Neutron Science and Instruments (IPN2003), Tsukuba, Japan [http://www.neutron.gov/mailman/listinf o/neutron]

27-31 October 2003 Ninth International Symposium on Radiation Physics. Cape Town, South Africa.

[http://www.medrad.tlabs.ac.za/isrp9.htm/]

31 October- 1 November 2003

UK-Japan Neutron Science Workshop (UKJ2003), Izura SPA (Pacific seaside), Japan

[http://www.neutron.gov/mailman/listinf o/neutron]

31 October- 1 November 2003

Neutron Detector Workshop (ND2003), Tsukuba, Japan [http://www.neutron.anl/mailman/listinf

o/neutron]

12-20 November 2003

A Practical Course in Molecular Microscopy, Center for Integrative Molecular Biosciences (CIMBio), The Scripps Research Institute (TSRI), La Jolla, California [http://nramm.scripps.edu/seminars/2003/cryoem/]

9-13 December 2003

International School on Crystal Growth and Characterisation ,La Pedrera, Rocha, URUGUAY [http://www.iscgcha2003.fg.edu.uy/]

15th March 2004

2nd Annual Biomaterials Workshop, Cranfield University, Shrivenham [http://www.cranfield-biomaterials.com]

22-24 August 2004

Satellite meeting on "Mathematical and Symmetry Aspects" (ECM-22). Budapest, Hungary, [http://www.lcm3b.unancy.fr/mathcryst/satellite.htm]

9-20 June 2004

Electron Crystallography: Novel Approaches to Structure Determination of Nanosized Materials, Erice, Italy. [http://www.crystalerice.org/2004/ElCryst 2004.htm]

9-20 June 2004

Polymorphism : Solvates and Phase Relationships. Erice, Italy, [http://www.geomin.unibo.it/orgv/erice/ bernstei.html

20-28 August 2004

32nd International Geological Congress, Florence, Italy [http://www.32igc.org/]

August 2005

XX Congress of the International Union of Crystallography, Florence, Italy [Carlo Mealli, email: [mealli@fi.cnr.it]

28 November - 2 December 2005

The dates for the 2005 International Conference on Neutron Scattering, Sydney, Australia. A website will be up and running shortly.



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