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CRYSTALLOGRAPHY NEWS

British Crystallography Association

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March 2001

Quarterly

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NEXT ISSUE OF CRYSTALLOGRAPHY NEWS

CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association. MSword97 documents (or earlier versions) or ASCII text files **may be sent on a PC disk or electronically,** (only small files < 500K please, image formats JPEG, GIF). Items may include 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, small ads, and advertisements for job vacancies in crystallography. Please ensure that items for inclusion in the **June 2001** issue are sent to the Editor to arrive before **26th April 2001**.

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President's Remarks

This newsletter may come as a bit of a shock. It represents a new departure for the BCA and was approved at the last Council meeting. Our newsletter serves two main purposes: to keep our members informed about crystallographic activities in the UK and elsewhere, but also to advertise British crystallography to other scientific communities. We often complain about the perception of crystallography in many academic departments as a routine service rather than an exciting subject in its own right (These people should just scan 'Nature' for a few weeks to have these illusions shattered!), and it was felt that a more professional looking Newsletter would help to enhance our image, as well as giving us more scope for keeping BCA members informed. Many other organisations have taken this route, and they seem to be satisfied that it is worthwhile. We will be printing an extra 500 copies for distribution to synchrotron sources, other crystallographic associations etc. (Extra copies are very cheap to produce.) It is, however, an experiment for one year; if it ends up being non-commercially viable, or there is a lot of hostility from members towards it, then we will look again.

The new look coincides with Jo Jutson taking over as newsletter editor. We all wish her well in this crucial and quite difficult job. Remember – the newsletter is only as good as its contributions. I would also like to repeat my thanks to her predecessor, Kate Crennell, for her immense efforts on behalf of the BCA.

Last month I mentioned Corporate Membership of the BCA as a way to proceed with a stronger partnership with equipment manufacturers and software developers in crystallography. We have now contacted a number of companies; we have had a number of enquiries and now have several such members with more on the way.

Finally, I would like to thank Gill Houston and her staff at Northern Networking (Euan Woodward, Claire Cresswell and Rona Munn) for their immense hard work, energy and efficiency in running the BCA office. A lot of these changes would have been impossible without them. I also know that Chris Cardin has greatly appreciated their help with the Reading Spring Meeting. Reading is shaping up to be an excellent conference, and I am looking forward to it. I hope to see you there.

Chris Gilmore
March 2001

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Note:
Dates in ( ) are when due for re-election or retirement. This list is also on the WWW at URL

http://bca.cryst.bbk.ac.uk/BCA/admin/coun.html

The first issue

This first issue of Crystallography News for 2001 sees changes in printer, format and editor but the content remains similar with a mix of technical articles, meeting information and reports and BCA matters. I have been a member of the BCA for about 12 years and served on the Industrial Group Committee for 7 years. I retired from full time employment at the end of 1999 and by Autumn 2000 I realised that although there were many advantages in retirement it was time to do something constructive. At this time I was approached and asked if I would consider becoming the next editor of Crystallography News and so here I am writing my first editorial.

I would like to thank Kate Crennell for all the help she has given me in producing this first issue. Kate has been an excellent editor for the past 5 years and is a very hard act to follow. Now I can appreciate all the time and effort that must have been involved during her time as editor. Thank you to everyone who contributed to this issue. The newsletter is what you the members and contributors make it and I hope that together we shall be able to continue the high standard that Kate has set.

Jo Jutson
March 2001

BRITISH CRYSTALLOGRAPHIC ASSOCIATION 2001 ANNUAL GENERAL MEETING OF THE BCA

Notice is hereby given that the Annual General Meeting of the British Crystallographic Association will be held on
Monday 9th April at 4.00 p.m. in the Palmer Building, Reading University

At this meeting we shall elect a Vice-President and a Secretary. The following nominations have been received.

For Vice-President
Professor Bill Clegg, proposed Mrs Kate Crennell, seconded Dr Frank Allen.
Professor Paul Fewster, proposed Dr Chick Wilson, seconded Professor John Finney and Dr Pam Thomas

For Secretary
Dr Christine Cardin, proposed Dr Hilary Muirhead, seconded Mr David Taylor. Nominations by e-mail should be sent to the Secretary **to arrive before 2 April, 2001.** Nominations for any post require a proposer and seconder, and an indication in writing that the nominee has agreed to stand for the post. Nominee, proposer and seconder should all be current BCA members.

Agenda
1. Approval of Agenda
2. Apologies for absence
3. Minutes of the last AGM (published in the December, 2000 issue of Crystallography News).
4. Secretary's Report to Council (published in this issue of Crystallography News).
5. Amendments to the Statutes and By-Laws (see December, 2000 issue of Crystallography News).
6. Northern Networking's Report.
7. Report of the Treasurer to include Presentation of the Accounts for 2000 and the Examining Accountant's Report.
8. Acceptance of the Accounts
9. Election of Officers and Ordinary Members of Council.
10. Appointment of Examining Accountant for 2001.
11. Any other business.

(It would be helpful if items for inclusion under 2 and 11 of the Agenda could be notified to the Secretary before the meeting).

Hilary Muirhead (Hon Secretary)

for BCA Vice President

Professor Bill Clegg,

University of Newcastle and Daresbury Laboratory

My research is mainly in chemical crystal structure determination, but also includes some synthetic work in coordination chemistry. I have particular interests in developing data collection methods, including diffractometer control, use of new X-ray sources, and especially synchrotron radiation, and have led the project to develop station 9.8 at Daresbury. Other interests include crystallographic education and training. I have previously served on the CCG committee, organised the BCA Spring Meeting in Newcastle in 1994 and a CCG session at the meeting in Leeds in 1997, and have been involved in the planning and teaching of the CCG intensive course every two years since it started in 1987. I have lectured at several BCA and CCG meetings since 1983.

Bill Clegg

Professor Paul Fewster,

Philips Analytical Research Centre and Imperial College

I have been a member of the BCA since its formation. I served on the Physical Crystallography Group Committee from 1983 until I retired as chairman in 1996 and the BNCC until it was dissolved. As secretary of the PCG, I served on BCA Council, CMMP and the Chemical Crystallography Group Committees. I joined the Industrial Crystallography Group Committee in 2000. I am very much in favour of bringing the common interests of all the BCA groups together.
After completing a PhD on biological structures and post-doctoral work, I joined Philips Research in 1981. For my work on X-ray scattering of semiconductors I received the Paterson Medal and Prize from the IOP in 1991 and a DSc in 1994. From 1992 to 1996 I was project leader of a research programme across four international Philips sites. I am presently Head of the Philips Analytical Research Centre and have held a visiting professorship in physics at Imperial College since 1996. Over the last few years I have been a member of the EPSRC Physics Evaluation Panel, College and prioritisation panels, IRC Selection Panel and the Chartered Physicist Committee of the IOP. I am a member of the Degree Accreditation Committee of the IOP and on the review panel for the XMAS beam-line at the ESRF. My research covers materials from proteins to metals, single crystal to amorphous materials, scattering theory and all types of X-ray instrumentation. Much of my work has been developed into commercial products and sold throughout the world, e.g. the Materials Research Diffractometer. I collaborate with many UK and international research groups and give numerous invited papers around the world. I have recently published a book entitled *X-ray Scattering from Semiconductors*, (Imperial College Press).

I would like to think that my enthusiastic support for UK science, both research and teaching in Universities and research in Industry would have some impact on the future of the BCA.

Paul Fewster

Acknowledgements
BCA Sponsors

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

Annual Report to the Council (2000)

From the Secretary

The present membership of Council is as follows:

President
Professor Christopher Gilmore

Vice-President
Dr Frank Allen

Secretary
Dr Hilary Muirhead

Treasurer
Mr David Taylor

Members
Dr Margaret Adams
Dr Jeremy Cockcroft
Professor Paul Raithby

Group Representatives
Dr Andrea Hadfield
(Biological Structures)
Dr Harry Powell
(Chemical Crystallography)
Professor Christopher Frampton
(Industrial Group)
Dr Chick Wilson
(Physical Crystallography)

Co-opted
Professor Michael Woolfson FRS
Professor Paul Barnes

Ex officio
Professor Michael Glazer
(Immediate Past President)
Mrs Kate Crennell
(Editor Crystallography News and Webmaster)
Dr Josephine Jutson
(Editor Elect Crystallography News)
Gill Houston
(Director of Northern Networking) attends meetings of Council.

An important event this year has been the appointment of Northern Networking to run much of the administration of the BCA. In addition they have been closely involved in the organisation of the Spring Conference.

The Council has met twice during the year: during the Spring Meeting at Heriot Watt University, Edinburgh and at Birkbeck College, London in October 2000. At the AGM in Edinburgh Professor Chris Gilmore was elected as President, Mr David Taylor was elected as Treasurer and Dr Margaret Adams, Dr Jeremy Cockcroft and Professor Paul Raithby were elected as Ordinary Members of Council. At the Council Meeting Professor Paul Barnes was co-opted to serve on Council and Dr Josephine Jutson was appointed as Newsletter Editor (from March 2001 issue). Chick Wilson has replaced Frank Allen as the BCA representative on the European Crystallographic Association (ECA).

In 2000 four excellent quarterly issues of Crystallography News were published. The coloured covers are very attractive and the Newsletter continued to make a small profit. A Colour Supplement on IUCrXVIII was published. Kate Crennell has been Newsletter Editor for five years. The BCA owes her a debt of gratitude both for the very high standard and for the fact that the Newsletter makes a profit.

During the year there were several meetings and workshops. All four groups have held meetings, including ones on 'Signal Transduction' (Birkbeck College, London), 'Computational Tools in Chemical Crystallography' (SmithKline Beecham Laboratory in Harlow), 'Non Ambient Diffraction Techniques' (Birkbeck College, London) and 'Artificial Structures' (University of Bristol). The Seventh Summer School in Protein Crystallography was held in Bristol.

Membership is healthy and many young crystallographers have received BCA bursaries to attend meetings and conferences, both in the UK and worldwide.

Some good friends and colleagues have died during the year including Paul Sigler, George Jeffrey and Arnold Beevers. Appreciations appear in Crystallography News.

We are looking forward to the BCA Spring Meeting at Reading. The Plenary Session is on Visualisation and the local organiser is Christine Cardin. The next BCA meeting will be held at Nottingham 25-28 March 2002.

Hilary Muirhead (Hon Secretary)

Chemical Crystallography Group AGM 2001

The Annual General Meeting of the Chemical Crystallography Group will be held on Sunday 8th April 2001 during the BCA Spring Meeting in Reading, starting at 12:30pm. Final details of the agenda, venue and other details will appear on the CCG web-site (http://bca.crystal.bbk.ac.uk/BCA/CCG/agm01.html). Items for inclusion in the agenda are invited and should be sent to the Secretary/Treasurer to be received no later than Friday 30th March 2001.

Nominations are invited for each of the posts of Chairman, Vice-Chairman and one ordinary committee member. Nominations must include the name of a proposer, a seconder and written consent (or e-mail) from the nominee that he or she is willing to stand. They should be sent so as to be received by the Secretary not later than Friday 30th March 2001.

The Chairman (Professor Guy Orpen) and Vice-Chairman (Professor Paul Raithby) retire after two years service and are not eligible for re-election to the same post. One committee member (Dr C.C. Wilson) retires after three years service and is not eligible for re-election to the same post. All three are eligible for election to other positions. All other officers continue in office.

Harry Powell
(Secretary/Treasurer)
MRC-LMB, Hills Road,
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e-mail hrp1000@cam.ac.uk

Physical Crystallography Group AGM 2001

The 58th Annual General Meeting of the Physical Crystallography Group of the BCA and the Structural Condensed Matter Physics Group of the IoP,to be held at the University of Reading, Sunday 8 April 2001, at 17:30 pm

Elections to the Committee
There are vacancies for up to two Ordinary Members of the Committee, and nominations for these are welcomed. Nominations should be sent to the Honorary Secretary:

Dr C C Wilson, ISIS, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX; email: C.C.Wilson@rl.ac.uk, by Friday 9 March 2001, or as soon as possible thereafter.

Dr M I McMahon is currently co-opted as the Structural Condensed Matter Physics Group representative to the CMMP Division of IoP and potential Committee members who would be appropriate to assume this important role are particularly welcomed.

Industrial Group AGM 2001

The 17th ANNUAL GENERAL MEETING of the Industrial Group will be held at the University of Reading on Tuesday, 10th April 2001 at 12.30 pm. Nominations are sought for the position of chairman and for two committee members to serve for three years from April 2001. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.
Dr P Holdway, Honorary Secretary, A7 BLDG, DERA, Farnborough, Hants, GU14 0LX. Tel. 01252 393117/392159, fax. 01252 397223, email: pholdway@dera.gov.uk.

Biological Structures Group AGM 2001

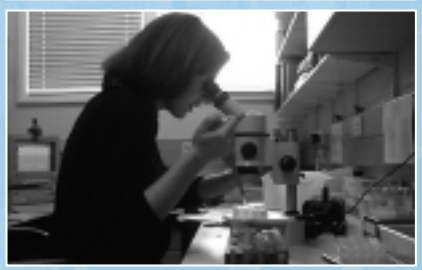
The Annual General Meeting of the Biological Structures Group will be held at the University of Reading on Monday 9th April at 12.30 pm

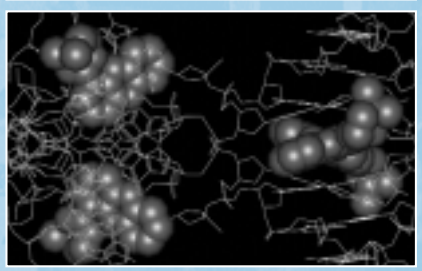
BRITISH CRYSTALLOGRAPHIC ASSOCIATION • SPRING MEETING • THE UNIVERSITY OF READING

BRITISH CRYSTALLOGRAPHIC ASSOCIATION

Spring Meeting

The University of Reading
7-10 April 2001





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BRITISH CRYSTALLOGRAPHIC ASSOCIATION • SPRING MEETING • THE UNIVERSITY OF READING

Chemical Crystallography Group Sessions

SATURDAY 7 APRIL
PLENARY SESSION:
Dr Sam Motherwell
(Cambridge Crystallographic Data Centre)
Visualisation of Molecular Interactions in Crystals

SUNDAY 8 APRIL 09.00 - 12.30:
CCG Session: Hot and Cold Structures
Professor Judith Howard
(Durham)
New Developments in Low Temperature Crystallography; Methodology and Applications

Dr Russell Morris (St Andrews)
Unusual properties of Zeolites Studied by Single Crystal Synchrotron X-ray Diffraction

Professor Philip Coppens
(SUNY, Buffalo)
Combining Crystallography and Photochemistry in the Study of Light-induced Metastable States and Transient Species

Dr Simon Parsons (Edinburgh)
Low temperature Crystal Growth

Chemical Crystallography Group Annual General Meeting (see separate notice in this issue).

SUNDAY 8 APRIL 14.00 - 17.30:
CCDC and Philips Prizes and Lectures followed by CCG / PCG / IG Oral Poster Session and Poster Exhibition

MONDAY 9 APRIL 09.00 - 12.30:
CCG/PCG Joint Session (1): Advanced X-ray Sources

CCG Speakers:
Professor Bill Clegg
(Newcastle/Daresbury)
New developments in Synchrotron Radiation

Dr Uli Arndt
(MRC-LMB, Cambridge)
Microfocus X-ray tubes for Crystallography

CRYSTALS WORKSHOP
Since CRYSTALS 2000 was demonstrated at Glasgow, we have received a lot of feed-back from old and new users. Some of this has been dealt with simply by e-mail and some of it has lead to improvements in the core program.

More operations have been automated and brought under the control of the graphical user interface, and a link has been provided to the Nonius Kccd data collection software and .INS and .RES files. As always, developing a graphical user interface discourages new users to look into the facilities not available from the GUI. Only a part of CRYSTALS's massive diversity is available from the GUI, and we are keen to make an opportunity to explain this diversity to a wider audience.

In addition, it is evident that users are intrigued by the way that the behaviour of the program can be tailored to meet individual needs through the macro or SCRIPT mechanism. These SCRIPTS can be used to simplify the repeated use of procedures, or to set up long and complicated experimental calculations. For example, Alain Penicaud, (in France) successfully wrote a SCRIPT to generate a series of trial models followed by refinement as a way of sorting out disorder in a C70 structure. All of the features in the GUI toolbars, menus and dialogues, and the layout of the screen itself, are controlled by SCRIPTS, which means that by editing a SCRIPT, the user can introduce their own ideas about how the program should look, feel or behave. In order to explain some of these items, we plan to hold a workshop at the BCA Spring Meeting in Reading to include:

- Demonstration of recent developments to the program, with special reference to evaluation and validation tools.
- Demonstration of the tools for manipulating the trial models, including model building, origin shifting, TLS regularisation, geometric regularisation, numbering and naming, hydrogen placement etc.
- Explanation of how SCRIPTS are written, and how they can be used to create teaching aids, and to automate frequently used crystallographic procedures,
- Hands-on experience of these and other features.

David Watkins

TUESDAY 10 APRIL 09.00 - 12.30:
CCG/PCG Joint Session (2): Diffraction at the Edge

CCG Speakers:
Dr Georgina Rosair
(Heriot-Watt)
Structural Chemistry from the Edge(s); an Introduction

Dr Madeleine Helliwell
(Manchester)
At the edge of microporous materials

Physical Crystallography Group Sessions

SATURDAY 7 APRIL,
PLENARY SESSION
Dr M.T. Dove
(University of Cambridge)
Visualisation of dynamics of disordered crystalline materials

SUNDAY 8 APRIL,
14:00 - 15:30
The **PCG Philips Physical Crystallography Award** and prize lecture, will be presented in a joint session with the CCDC/CCG prize winner.

SUNDAY 8 APRIL,
16:00 - 17:30
The joint PCG/CCG/IG **Oral Poster Session** will be held following the award session. **All** poster presenters are "invited" (with arm twisting) to deliver a 2 minute snapshot of their poster to encourage people to have a closer look in the poster session.

SUNDAY 8 APRIL,
17:30-18:00
Annual General Meeting of the Physical Crystallography Group (also the Structural Condensed Matter Physics Group of the IoP). See elsewhere for agenda and details.

MONDAY 9 APRIL,
09:00 - 12:30
Joint sessions on "**Advanced X-ray sources**" with the CCG:
(I) New Sources. This session will cover new radiation sources both in the home laboratory and at national facilities - design and application to real problems.
PCG Organisers - Steve Collins (S.P.Collins@dl.ac.uk) & Dave Allan (dra@ph.ed.ac.uk)

Speakers:
Mike Poole (Daresbury)
DIAMOND design
Colin Norris (Leicester)
Science on DIAMOND
Bill Clegg (Newcastle)
Single crystal diffraction using SR
J Schneider (HASYLAB)
Free-electron laser X-ray sources
Uli Arndt (Cambridge)
Microfocus X-ray tubes for crystallography

MONDAY 9 APRIL,
13.30 - 15.30
COHERENCE WORKSHOP
In a timely bid to reflect an important trend in x-ray science, the Physical Crystallography Group are holding a FREE* workshop on the topic of Coherence and Crystallography at the Spring Meeting of the British Crystallographic Association in Reading.

If you are a crystallographer in any research area – whether Laboratory-based or synchrotron based – this Workshop could be for you. With the many advances in x-ray sources, particularly with 3rd-generation x-ray sources such as E.S.R.F, the opportunities, and sometimes difficulties, presented by increased coherence can hardly be ignored.

Whether or not you know your lateral coherence length from your elbow, come along and participate in this informal workshop, which comprises two short tutorial talks - one on general aspects of coherence by Dave Laundy and the other on implications for biological crystallography by Colin Nave - and short contributions/ discussion points/questions from participants, such as:

What determines the final profile in a diffraction experiment?
Do coherent speckle experiments give useful information?
What determines the lateral coherence in an experiment – the sample or the source?
Phase-contrast imaging – the wheel re-invented?

To participate in the Workshop, register on-line at http://www.isis.rl.ac.uk/Crystallography/coherence.htm and gain FREE entry to the PCG Coherence prize-quiz. {Winner and prize TBA at the Workshop}

For further information, and/or to contribute a discussion point, comment or question to the Workshop, please contact:
Dr. Pam Thomas, Dept of Physics, University of Warwick,
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Tel. 02476-523354
Fax. 02476-692016
E-mail:
p.a.thomas@warwick.ac.uk

*Workshop is free to registrants of the British Crystallographic Association Spring Meeting. Details of this meeting can be found at http://bca.cryst.bbk.ac.uk/BCA/meets/BCA01.html

TUESDAY 10 APRIL,
09:00 - 12:30
Joint sessions on "**Advanced X-ray sources**" with the CCG:
(II) Diffraction at the Absorption Edge. This session will deal with new opportunities for experiments at X-ray absorption edges - the hows and whys.

PCG Speakers
Brian Tanner (Durham)
Resonant diffraction from multilayers
Des McMorrow (Riso)
Diffraction studies of charge/spin/orbital ordering
V E Dmitrienko (Moscow)
Forbidden reflections and partial structure solution using anisotropic anomalous diffraction

Industrial Group Sessions

BASIC POWDER DIFFRACTION WORKSHOP (SUNDAY 8 APRIL & MONDAY 9 APRIL)

This one and a half day course has been constructed with a special concern for the many people now working in X-ray Powder Diffraction who are relatively new to the field. There are no special pre-requisites for taking part, other than a general technical background, but a little hands-on experience of XRPD would help.

INTRODUCTION TO CRYSTALLOGRAPHY (SUNDAY 09:00 - 12:30 8 APRIL)
Jeremy K. Cockcroft,
Birkbeck College London

This session will cover the basic crystallographic principles underpinning powder diffraction with emphasis on the factors that determine the position and intensities of the peaks in a powder pattern. In addition, some of the crystallographic factors affecting profile line shape will also be discussed. A brief overview of crystallographic symmetry and its affect on powder data will be covered. Having dealt with the basic principles, we will then discuss the principles and practice of indexing, unit cell refinement, and space group determination of our powder diffraction data.

POWDER DIFFRACTION INSTRUMENTS (SUNDAY 14:00 - 17:30 8 APRIL)
Judith Shackleton, Manchester Materials Science Centre

In this session we will investigate powder diffraction geometry. We look at the various components of the diffractometer, what they do, how they work and how we make the optimum choices. We will also discuss the choice of X-ray tubes, the anode and tube focus as well as the characteristics of various types of detectors. The selection of data collection conditions (step size, counting time etc) and the importance of good sample preparation will also be described.

PHASE IDENTIFICATION (MONDAY 09:00 - 12:30 9 APRIL)
John Faber, Principle Scientist International Centre for Diffraction Data

This session will give an overview of the history of phase identification and the development of the ICDD powder diffraction file (PDF). Methods of identification and characterisation of crystalline substances by use of the PDF will be covered. The importance of gathering good quality data and the use of new computer aided search methods will be demonstrated. The content is designed for both beginners and experienced users of the Powder Diffraction File.

For further information, please contact:
Dave Taylor,
35 Birchley Road,
Billinge, Wigan,
Lancs. WN5 7QJ
tel. 01744 893108,
email: djtaylor@lineone.net

WHY INDUSTRY USES CRYSTALLOGRAPHY (MONDAY 9 APRIL)

Crystallography has wide application in many of our manufacturing industries. This session will give a series of overviews of the value that crystallography brings to a selection of these industries. While we hope these surveys will be interesting in their own right, we also intend that they spark some ideas across traditional industrial boundaries. Presentations on the following industries are planned:

Aerospace, Pharmaceuticals, Electronics & Minerals.
The session will begin with:
The Alun Bowen Industrial Lecture
'Crystallography in the Aerospace Industry'
Colin Small, Rolls Royce
For more information, contact:
Steve Norval, ICI plc, Science Support Group,
Wilton Centre, PO Box 90,
Wilton, Middlesbrough TS90 8JE,
tel. 01642 432005,
fax. 01642 432244
email: steve_norval@ici.com.

NEW & FUTURE POSSIBILITIES IN POWDER DIFFRACTION (TUESDAY 10 APRIL, 09:00 - 12:30)

The programme highlights some aspects of instrumentation and methodology in powder diffraction that have seen recent advances and explores what we should expect to see in the future.

The X'Celerator: a breakthrough in powder diffraction
Dr Anna Widdowson,
Philips Analytical

Hardware & Software Innovations
Dr Gÿtz Menges, Bruker AXS Gmbh

New Developments with the PDF Database
Dr John Faber, ICDD

Rietveld Refinement: Past, Present, & Future Possibilities
Jeremy Cockcroft,
Birkbeck College

The session will include two further presentations; details will be posted on the Industrial Group Web pages as soon as they become available.

For more information, contact: Steve Norval.

Industrial Group Posters
Posters are invited for display at the Spring Meeting. As an extra incentive to your participation, in addition to the acclaim that your poster will no doubt bring, the Industrial Group is offering a magnificent prize of £50 for best poster.

Some guidelines follow for what we would prefer to see in our posters and our adjudicators will work from these.

Posters are encouraged that:

- are relevant to industry (including some background and value of the work to industry)
- have clear aims, results and conclusions
- concentrate on telling the story, rather than fine detail
- are not an advertisement for a commercial product

There will be an opportunity to give a brief oral presentation of the content of each poster.

Biological Structures Group (BSG) Sessions

SATURDAY 7 APRIL,
2P.M - PLENARY SESSION
Looking at structure.
Professor Rod. E. Hubbard (York)

BSG SESSION 1.
HOW MAD CAN YOU GET?
(SUNDAY 8 APRIL, 14.00 - 17.30)
This session will cover all experimental aspects of structure determination by the MAD method from selenomethionine expression to locating the sites as well as novel developments in the field such as the exploitation of the anomalous signal from biologically occurring elements.

Expression of selenomethionyl-substituted proteins.
Neil McDonald (ICRF/Birkbeck)

Exploiting anomalous signal, experimental methods of phasing macromolecular structures: methods, pitfalls and perspectives.
Sean McSweeney (EMBL/ESRF, Grenoble)

Xenon and soft X-ray MAD.
Pierre Rizkallah (Daresbury Laboratory)

Methods for locating the anomalous scatterers in macromolecular structures.
Thomas Schneider (Gottingen)

Phasing on anomalous halides.
Zbigniew Dauter (Brookhaven/Frederick, USA)

BSG ORAL POSTER PRESENTATIONS
(SUNDAY 8 APRIL, 11.00 - 12.30)

BSG SESSION 2.
STRETCHING THE LIMITS - PROTEINS AT ATOMIC RESOLUTION.
(MONDAY 9 APRIL, 09.00 - 12.30)
This session will look at atomic resolution studies of proteins both as a tool for solving new structures and for mechanistic studies of enzymes. Complementary developments in the neutron field will be covered.

High resolution data collection: optimising the chances.
Elspeth Garman (Oxford)

Protein structures at atomic resolution.
Keith Wilson (York)

Protons in proteins: how to see hydrogen atoms at medium resolution.
Dean Myles (EMBL/ILL, Grenoble)

Crystallography at subatomic resolution: the aldose reductase structure at 0.66 Angstrom resolution.
Alberto Podjarny (Strasbourg)

Enzymatic degradation of high-explosives at atomic resolution.
Peter Moody (Leicester)

BSG SESSION 3.
HOT STRUCTURES
(MONDAY 9 APRIL, 13.30 - 15.30).

Acetylcholine Binding Protein (AChBP), a homologue of the ligand-binding domain of the nicotinic acetylcholine receptor.
Katjusa Brejc (Netherlands Cancer Institute, Amsterdam)

Structure of a collagen - and perlecan-binding fragment of nidogen.
Erhard Hohenester (Imperial, London)

Two metal binding beta-jellyrolls: oxalate oxidase and auxin receptor.
Eui-Jeon Woo (Queen Mary, London)

Bifunctionality and the structure of mammalian sperm beta-acrosin.
Becky Tranter (Bristol)

Crystal structure of the Holliday junction-resolving enzyme T7 endonuclease I at 2.1 Angstroms resolution.
Jonathan Hadden (Leeds)

An unsuspected covalent intermediate in the epimerisation of carbohydrate reveals a new class of mechanism.
James Naismith (St Andrews)

THE BRAGG LECTURE (MONDAY 9 APRIL, 17.00 - 18.00).
Bragg reflections illuminate the structures of some perfidious viruses. Dave Stuart (Oxford)

The North West Structural Genomics Centre

Following the recent North West Science Review, funding has been allocated for the first UK academic structural genomics effort. The North West Structural Genomics Centre (NWSGC) consortium will consist of several north west universities (Manchester, UMIST, Liverpool and John Moores), AstraZeneca and Daresbury Laboratory. The NWSGC members bring together expertise in protein crystallography, human pathogens, membrane proteins, metalloproteins and the internationally recognised Liverpool School of Tropical Medicine. The centre will be based around a dedicated high throughput Multi-wavelength Anomalous Dispersion (MAD) beamline on a high field multipole wiggler on the SRS, Daresbury Laboratory. The initiative aims to establish the technology for high throughput structure determination in the UK.

The centre will target pathogen genomes, and more specifically proteins likely to mediate host pathogen interactions. This is an area of particular strength in the research groups in the north west of England. The elucidated structures are expected to provide insights into the workings of these biological molecules. It is likely that they will be important for rational drug design and the diagnosis and treatment of disease, as well as in the advancement of the basic principles of biology. Our ultimate aim is to improve the understanding of host pathogen interactions, leading to the development of more effective drugs.

Details for the NWSGC can be found at http://www.nwsgc.ac.uk

Samar Hasnain
CLRC Daresbury Laboratory

Beamline BM14 at the ESRF, Grenoble

Beamline BM14 at the ESRF - one of the premier MAD protein crystallography beamlines in Europe - has recently been purchased by the UK Research Councils (MRC, BBSRC and EPSRC) in collaboration with the EMBL Outstation in Grenoble. Initially, BM14 will be jointly operated by UK and Spanish consortia as a Collaborative Research Group (CRG) in conjunction with the ESRF, and will transfer to sole UK management in 2003.

The intention of the steering committee is to provide rapid access to BM14 on a per project basis with beam time being scheduled within 6-8 weeks of the initial proposal being submitted. This should particularly help smaller research groups to gain access to facilities at the ESRF. In addition to fostering the use of MAD techniques in UK laboratories, the beamline will be further developed with the aim of establishing automated methods of sample changing, crystal location and crystal alignment.

Applications for beam time are now invited from all members of the UK research community (regardless of funding source) and can be made by visiting the BM14 UK web site (http://www.bm14.ac.uk/bm14/proposal.html). The proposal form is very short and decisions will be made by an independent Review College within about one week of submission. Priority will

be given to MAD experiments, although all projects that would benefit from the facilities at BM14 will be considered. Researchers interested in applying for EMBL time on BM14 should contact EMBL, Grenoble directly in the first instance and then submit proposals through the BM14 UK web site. The Spanish consortium will operate its own beam time allocation procedure. For further information please go to the BM14 UK web site (http://www.bm14.ac.uk/) or send an email to enquiries@bm14.ac.uk.

David Stuart, Oxford University
Guy Dodson, York University and NIMR, Mill Hill
Neil Isaacs, Glasgow University
Andrew Leslie, Cambridge University
Simon Phillips, Leeds University

ILL News – Update on ILL diffraction instruments

The Institut Laue-Langevin, in Grenoble, France, provides a comprehensive range of neutron diffraction facilities and in-house user-friendly expertise for crystallographic experiments in physics, chemistry and biology. For further information see http://www.ill.fr/dif & http://www.ill.fr/lss.

Latest News

D10: For those really tricky crystallographic problems, where conventional high-flux single-crystal diffractometers still leave you wondering, you might consider trying D10. With optional energy analysis, very low intrinsic background, large wavelength range and sturdy sample table, it gives you the flexibility to explore reciprocal space to high resolution over a wide dynamical range under extreme sample environments, often in full four-circle geometry. It is the instrument of choice for detailed study of phase transitions, with appeal not just to physicists but also to chemists, mineralogists, and others. A new addition in 2001 is a lifting detector support to allow inclination of the 80x80 mm2 position-sensitive detector by up to 30° to the equatorial plane for greater reciprocal-space access with bulky or heavy sample environments.

VIVALDI (**V**ery **I**ntense, **V**ertical-**A**xis, **L**aue **Di**ffractometer) is on schedule for installation in the spring of 2001. The vertically-mounted cylindrical image-plate detector will accept an Orange cryostat and offer temperatures from 30 mK to 600K for rapid study of phase transitions, refinement of reasonably large structures to atomic resolution, and immediate investigation of 'hot' structures. Further details on these and other instruments can be found under http://www.ill.fr/YellowBook.

How to apply for neutron beam time

Our deadlines for beam-time applications are 15 February and 31 August. Accepted proposals submitted by February will receive beam time in the second half of the year, and those submitted by August in the first half of the next year. Invited scientists affiliated to the ILL member countries are assisted with travel costs and subsistence. For further details please see http://www.ill.fr/SCO. For hot topics or new users there is the possibility to apply for Director's discretionary time during the year.

S A Mason and G J McIntyre
Institut Laue Langevin
1 February 2001

Spreadsheet Library

Library of Excel Routines for Diffraction and Crystallography

The Industrial Group has set up a library of Spreadsheet routines running on Microsoft Excel.

The first release was made available for download on 19 Jan 2000. The files can be downloaded in a single zip file or just the individual files you require from:

http://www.ccp14.ac.uk/ccp/web-mirrors/bca-spreadsheets/

If you have developed an XRD/Crystallography spreadsheet routine you wish to share then please e-mail a copy to djtaylor@lineone.net

USEFUL WEB SITES

A Science Forum entitled "Scientific Advice and Public Confidence" can be found on the Citizen Portal website: http://www.ukonline.gov.uk.

Next Wave at http://nextwave.sciencemag.org/uk is a useful site if you need career advice. It also has areas devoted to science policy, job market news, job hunting, career training, Postdoc work, salary surveys, Postdoc and Faculty issues.

Honary Fellow of the Royal Society of Chemistry

Professor Jack D. Dunitz of the Swiss Federal Institute of Technology, Zurich has been made an Honorary Fellow of the Royal Society of Chemistry. Jack studied chemistry at Glasgow University, (Ph.D. 1947) and held research fellowship at Oxford University (1946-1948, 1951-1953), the California Institute of Technology (1948-1951, 1953-1954), the U.S. National Institute of Health, Bethesda MD (1954-1955), and the Royal Institution, London (1956-1957), before taking up a professorship at the ETH-Zürich, a post that he held until his retirement in 1990. He has held Visiting Professorships in the United States, Israel, Japan and the United Kingdom, has been elected to membership of several learned societies, and has received several awards for his work. He has written more than 300 scientific papers and is the author of 'X-Ray Analysis and the Structure of Organic Molecules' (Cornell University Press, 1979; Verlag HCA, Basel, 1995) and 'Reflections on Symmetry in Chemistry...and Elsewhere' (with E. Heilbronner, Verlag HCA, Basel, 1993).

OBE awarded to Professor R. Nelmes

Congratulations to Professor Richard Nelmes, University of Edinburgh and Senior Visiting Fellow at CLRC, on the award of an OBE in the New Year Honours List for services to science. Richard leads groups from the University of Edinburgh based full time at both ISIS (CLRC Rutherford Appleton Laboratory) and the SRS (CLRC Daresbury Laboratory). Over the past decade he and his colleagues have developed many new techniques and facilities for studying crystal structures and transitions at very high pressures, using diffraction methods with neutron and synchrotron beams.

Most recently, Richard has led a successful £7m bid to the Joint Infrastructure Fund to set up a Centre for Science at Extreme Conditions (CSEC) based in Edinburgh. This will provide the extensive laboratory-based facilities needed to make the most of the opportunities provided by modern neutron and synchrotron sources, and will be particularly effective when diamond is in operation. CSEC will bring together neutron and synchrotron facility users in five departments in Edinburgh to tackle a wide range of extreme conditions science including research into novel materials made at high pressures and temperatures, the use of pressure to tune and optimise applied electronic properties, materials and processes for extreme conditions engineering, earth and planetary science, high-pressure biology, and fundamental condensed-matter physics.

Extracts from an article which was first published in the CLRC 'Labnews' for January 2001. I am grateful for permission from RAL Press and Public relations for permission to reproduce it here. The photograph is copyright CLRC reference no (96RC3864).

Industrial Group Award 2000 Dr David Dyson

(see also report of the IG Autumn Meeting 2000)

David Dyson receiving his award from Chairman Steve Norval

David Dyson was presented with an Industrial Group Award during the 2000 Autumn Meeting at Roche Discovery, Welwyn. David has been associated with BCA Industrial Group from its inception. He has contributed widely to group activities and served on the committee as an ordinary member, vice-chair and chair between 1989 and 1996. David's involvement with crystalline materials and industry began when he joined G.E.C from university, characterising reactor graphite materials. That developed an interest in high temperature studies, crystallite size and strain using camera and diffractometer methods.

18 months later, David returned to his native Yorkshire to work with United Steel Companies, which later became British Steel. This brought together interests in electron and x-ray diffraction that David has pursued ever since. Early studies covered phase analysis in oxide systems that led to the identification of a number of new phases appearing in the powder diffraction file. In the 60s, he developed the diffractometer method for analysing dust on air filters and contributed to the MDHS standard used since for environmental monitoring.

David was one of the first people in industry to recognise the importance of computers in the XRD laboratory for data collection and analysis. A large suite of programs followed covering a variety of aspects of his work. He developed means for the quantitative analysis of a number of products in the steel industry and contributed to development of profile fitting methods. He became very interested in the effects of solid solution and preferred orientation, both of which are common in the steel industry. David has also contributed to British Standards in Texture Analysis of steels. He was responsible for setting up the BS in the early 70s and developed the software. The use of ODF saw him talking to and advising suppliers on how to output the data.

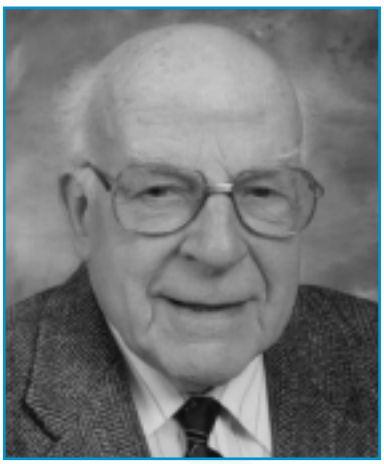
There was a series of BS reports on electron diffraction that subsequently appeared as a book - still selling world wide (He says it needs updating and re-issuing!) This introduced him to single crystal work and geometry of diffraction with the stereographic projection became one of his most useful tools. Installation of a 1000KV HVEM at Rotherham enabled him to study phase transformations and orientation changes in situ during straining and at high temperatures via diffraction studies.

An area of David's activity that has become very familiar in recent years is his strong interest in quality assurance, especially in relation to NAMAS / UKAS. Several of us have benefited from his regular and thorough assessment visits!

There are inevitably many important things missed here from David's many contributions to industrial crystallography. He has published well over 100 papers and given many lectures both at home and abroad. But I hope it will be very clear that David is a very worthy a recipient of this award.

Dr Steve Norval

Dr C. Arnold Beevers



With the death of Dr C. Arnold Beevers, Reader Emeritus in Crystallography at the University of Edinburgh on 16 January, 2001, we have said farewell to a great man, who was scientist, teacher, inventor, humanitarian and humorist in a rare combination. Arnold was born in Manchester on 27 May, 1908, but his family moved shortly thereafter to Liverpool, a city of which he was always proud. His father was a master tradesman, whose work included the installation of the glass roof of the Lever factories. He obtained a B.Sc. in Physics from the University of Liverpool in 1929, and a D.Sc. in 1933. While there, he was greatly influenced by Professor Lionel Wilberforce, whose well-designed springs and clamps Arnold never tired of demonstrating. After graduation, he was asked to set up work in the relatively new subject of X-ray diffraction together with Henry Lipson, a colleague and friend for many years. The two of them made frequent trips (sometimes by bicycle) to the University of Manchester to get advice from Lawrence Bragg, and Arnold eventually moved to a post there. After a short appointment at Hull, Arnold was appointed in 1938 to the Dewar Fellowship in Crystallography. This was a post offered jointly by the Departments of Physics and Chemistry at the University of Edinburgh, and he was elected Fellow of the Royal Society of Edinburgh later that year. And in Edinburgh he remained, coming into his office in the Chemistry Department for the last time less than two months before he died.

As a young adult, Arnold, like Kathleen Lonsdale, felt drawn to join the Religious Society of Friends (Quakers) and his deep faith in and with that body greatly influenced his approach to science and to life. He was unswervingly committed to humanitarian causes, and in particular to world peace, and he strongly disliked any form of superstition or other obscurantism, and any sort of pomposity. His life was touched by tragedy, especially the severe dementia which overtook his wife Marjorie in the late 1950's, and which grew ever worse until her death in 1992. Sadly, a similar problem affected Yvonne, his second wife, who died in 1998. In these circumstances, his never-failing sense of humour was all the more remarkable.

Arnold's scientific contributions were many. From his early days, he is most remembered now for the Beevers-Lipson strips, and the technique by which they reduced the huge calculations of three-dimensional Fourier summations to sums of manageable one-dimensional ones. These attractive boxes of strips of card were produced in great quantity until the digital computer became generally available in the late 1960's. The technique is still used in many computer programs. Arnold's earliest structural publication was a correct and beautiful reinterpretation of the structure of beryllium sulfate tetrahydrate as interpenetrating tetrahedra of $Be(H_2O)_4^{2+}$ and SO_4^{2-} ions. Previously, a remarkably imprecise treatment had found that the sulfate ions were planar! Arnold rapidly became involved in determinations using Fourier methods and the new Patterson method; important examples were the alums, copper sulfate pentahydrate, and particularly the so-called ß-alumina, $NaAl_{11}O_{17}$, which he published with the late Dr Marion Ross. Originally studied as a troublesome impurity in Al_2O_3 production, it is now an important solid-state ionic conductor, and two sites in the structure are known as Beevers-Ross and anti-Beevers-Ross sites.

Arnold's arrival in Edinburgh was soon followed by the outbreak of the Second World War. As a conscientious objector, he was sent to assist Professor Norman Dott at the Western General Hospital in his work on electroencephalography. Arnold threw himself enthusiastically into this work, particularly as it threw light on the nature of sleep, and this interest remained with him for the rest of his life.

After the war, Arnold joined the Department of Chemistry as a member of staff, and built up an X-ray diffraction laboratory there, mainly with equipment he had designed himself. His generators and cameras were characteristically robust and precisely engineered. The arrival of Professor E.L. Hirst and the growth of his carbohydrate group encouraged Arnold to investigate the then daunting structures of sugars, and ones he studied included glucose, and sucrose in the form of its sodium bromide adduct.

As a teacher, Arnold gave lectures of a highly individual nature, which have remained in the memories of generations of students. As an experimenter, he delighted in

demonstrations, although they did not always behave for him. One lecture ended uproariously as an explosion he had attempted to demonstrate finally worked in the hands of the technician who was removing the apparatus. Happily, no serious damage was done to the technician or anyone else! Younger colleagues were surprised (to say the least) to see Arnold showing the bones of his hand to visitors by using the direct beam from the lab X-ray generators. Again, he always seemed to get away with it. His crystallography lectures generally featured safer equipment, including the collection of plasticene elephants he used to occupy the sites of a lattice. He also had a large assortment of collecting boxes for Dr Barnardo's Homes for this purpose, frequently pointing out that this was an excellent charity and that the boxes had another useful function! He was honoured one year by a song from the honours students, showing that they had learned at least something from him:

Twinkle, twinkle, little star
How I wonder how you are?
For you have five points, I see,
And I know that cannot be.
You must be point group 33
A new system of symmetry!

Possibly his most lasting impact as a teacher was his teaching of chemistry for dental students over many years. In 1946, he published an elegant interpretation of the structure of fluorapatite, the ideal bone and teeth mineral, showing the function of the fluoride ions in holding it together. Thereafter he became devoted to the cause of improving dental health by adding fluoride to drinking water supplies which were deficient in it. He often spoke at rallies on this subject, cheered on by his students, and was once caught in a photograph by the Scotsman with raised fist, in a most unpacific manner! When he retired in 1978, the Edinburgh University Dental Society gave him a life membership of which he was always very proud.

Arnold was for many years active in the Edinburgh Cripple Aid Society. He was in much demand as a helper, particularly as Master of Ceremonies at plays and concerts. An epileptic seizure affecting a leading lady never fazed him, and he could immediately take over, often getting the audience engaged in community singing. He displayed this ability equally at international scientific meetings. Particularly famous at home and abroad was his version of "My Bonnie lies over the Ocean" in which the singers must stand up or sit down on each word beginning with "b". Generally, by the third chorus, even a group of scientists were coping with all the "bring backs"! At one international school, he produced a song for the final dinner, which took place after a particularly long and boring lecture. At the end of the song, Arnold remarked brightly, as no one else would have dared, "I wrote that in Professor H****'s lecture this morning. Had he gone on any longer, there would have been even more verses!"

The involvement with handicapped people was very important in Arnold's last major scientific contribution, what are now known as Beevers Miniature Models. Arnold moved away from structure determination after 1960, as he was never really happy with the advent of the digital computer; for the first time, he was being asked to use equipment which he could not fully comprehend and design himself. He sensed the need for accurate ball-and-spoke models on a scale much smaller than that of the inch to Ångstrom models then available, and developed precision drilling machines to enable the scale to be reduced to 1 cm per Ångstrom. After some experimentation, he fixed on the 7mm perspex spheres and 1mm steel rod now used, being determined that the models must be both accurate and elegant. Typically, he published his methods and would have no truck with the idea of a patent, which he saw as unfairly denying public access to his ideas and methods. The calculations required for drilling, he carried out manually, using a Wulff net for his stereographic projections. From the beginning, much of the work was carried out by handicapped workers, including at one time Brian Wilson, the world's longest surviving patient on renal dialysis (as listed in the Guinness Book of Records!). These workers clearly took great pride in their work, which have gone all over the world, to institutions ranging from a school in Port Moresby, New Guinea, to I.B.M. Research. Over the years, the Models were taken over by the University, and Arnold accepted that lesser mortals would have to use the computer even for drilling calculations. He was actually pleased to see himself eventually on a website!

The Beevers Miniature Models Unit continues, showing that he was right that computer modelling would not replace completely the elegant, permanent model in museums, teaching or research. Arnold is survived by Lois and John, his daughter and son, by four grandchildren and five great-grandchildren. Many former students and colleagues world-wide have joined in sending them their sympathy and their happy memories of a great and kind man.

Robert and Sheila Gould

Non-destructive determination of mechanical stresses at ILL

The high penetrating power of neutrons make them well suited to measurements deep inside matter. One application that takes advantage of this property is the neutron strain imaging technique for the non-destructive determination of mechanical stresses. Any engineering component is stressed to some extend, which can have positive or negative influence on the properties of the component. Therefore its determination is of great importance. The advantage of the neutron technique is that it is applicable to small as well as to large specimens and that no special sample treatment is necessary before an experiment. Newly developed materials, samples from the production line or after wear are equally good candidates for the neutron strain imaging technique which makes it attractive to both the scientist and the mechanical engineer. Some examples which demonstrate the range of applications are: welds, interfaces, coatings, hardening, fatigue and composite materials.

At the ILL stress determination is done on the D1A diffractometer. It is applicable to specimens from about 1 cm3 size up to half a meter in length and weights not exceeding 80 kg. A stress-rig which works up to 15 kN in tension and compression is available. The latest development on the instrument is a new beam optics that provides much higher lateral resolution for interface and surface measurements. This is a unique feature for this type of instrument and makes it suitable for investigations of surface treatments such as shot peening or coatings, especially on materials containing heavy elements or welds which show a thin heat affected zone and high stress gradients.

Computer calculations are frequently used to optimize components and manufacturing processes. But they often have to use simplified models to achieve reasonable calculating times; so for confirmation measurements are indispensable. Achieving absolute values for the calibration of models is another important point for measurements. The results from neutron strain imaging can be compared directly with finite element simulations since both determine strain values. An example where the neutron experiment helped to verify the finite element model and optimize the manufacturing process was a measurement on roller straightened railway rails, recently performed at ILL.

Roller straightening is the last step in the production of a rail. Therefore it determines the final mechanical properties of a rail i.e. straightness, flatness of the running surface and residual stresses. Rails used for goods trains or in curves are hardened by applying a heat treatment after straighten them. It must be insured that this treatment does not introduce additional tensile stresses into the rail, since they allow crack initiation and may support crack propagation. Two rails from production were investigated: a roller straightened rail and an additionally hardened one. Two 0.5 m long rail sections were chosen for the experiment and measurements were performed on a cross section as shown in fig 1. The longitudinal strain component of the two rails is plotted in fig. 2. Position 0 mm is the surface of the railhead, 170 mm the foot.

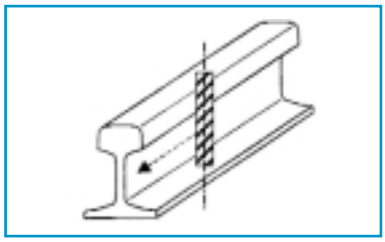


Figure 1. The rail and the plane along which the measurements have been performed. The arrow shows the direction of the longitudinal strain component.

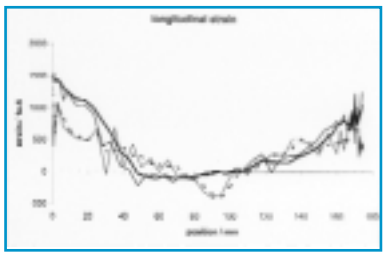


Figure 2. The solid curves show the evolution of the longitudinal strain component in the head hardened rail and the dotted lines in the non-treated rail. There is no negative influence of the hardening process on the strain-, and therewith the stress distribution in the rail.

The measurements indicate that the strain-, and therefore the stress- distribution in the hardened rail is not very different from the not heat treated one, which is the desired result. (This experiment was part of the thesis work of Gerald Schleinzer of the Institut für Mechanik, Montanuniversität Leoben, Austria)

A new instrument

The present strain imaging set-up at ILL is somehow inconvenient since the space available for samples is limited. Due to the importance of the technique ILL has decided to build an instrument dedicated to the determination of (residual) stresses. The work on the new instrument has already started and is now continued in collaboration with the University of Manchester, jointly funded by the ILL under the ILL Millennium program, and the EPSRC. The new instrument will be constructed and commissioned

over the next four years. The objective is to enable measurements in samples of up to 1000 kg weight and up to between 1.5 m and 2 m length. A unique sample table - a hexapod - will position the specimens to high accuracy and allow scans in any direction. A new super mirror neutron guide and a double focusing monochromator will provide between 3 and 5 times the intensity of the present instrument and allow high-resolution measurements at the same time. We are looking forward to the new instrument since it will extend the range of applications tremendously in research and for industrial use.

Thilo Pirling
Institut Laue Langevin, Grenoble
1 February 2001

MAKING MAPS OF MAGNETISM

Article reprinted courtesy of CLRC Rutherford Appleton Laboratory

MAPS is ISIS's new neutron scattering instrument designed to investigate single crystal samples. After its first cycle of scientific commissioning it is already breaking new ground in furthering our understanding of magnetic materials.

The behaviour of large and complex aggregations of elementary particles or atoms cannot be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity, entirely new properties appear and understanding the new behaviours requires fundamental analysis. The parallels between high energy physics and condensed matter physics is especially strong in the studies of magnetism and the strong correlations between atoms. Here particle physics merges with condensed matter theory.

Dr Alan Tennant, a Research Fellow at Wadham College, Oxford, was one of the first users of the new machine; he describes it as *"a revolutionary step-forward for neutron scattering." "Neutron scattering is unique in being the most direct and versatile way to see quantum mechanics in action, with all of the correlations and interactions between atoms in a material becoming visible,"* he said. *"Quantum mechanics gives the fundamental rules of how atoms interact, and the richest set of rules are encapsulated in magnetism. Studying model magnetic systems provides insight into the complex rules that govern everyday behaviour. The huge advantage of the MAPS instrument is the collection of a 3-dimension volume of data that reveals the whole picture of the atomic correlations in one snapshot with unprecedented detail."*

Some stunningly beautiful data from the first few weeks of operation are demonstrating the full power of the MAPS position sensitive detector array that divides a 16.5 m_ area into some 150,000 individual pixels. The 500Mbytes of data collected per measurement are analysed by powerful visualisation and other software that provides experimenters with unprecedented freedom to group individual pixels together to optimise the instrument's resolution for their particular experiment. It is almost as though they are reconstructing the instrument for every new measurement, and furthermore they can continue to do this even after the actual data collection has ceased.

Chris Frost in front of the vast 16m MAPS position sensitive detector array, developed at ISIS by Julian Norris, Nigel Rhodes and colleagues.

In its first period of operation MAPS has already revealed new excitations in a previously well studied material, demonstrating that novel instrumentation leads to new scientific avenues and opportunities.

The users were greatly excited that the new generation of instruments, like MAPS, demonstrates that the performance is no longer necessarily defined by the quantity of neutrons, but also by the progress in the technology incorporated in their designs. Technological advances are driving neutron instrumentation forward, allowing the collection, manipulation and visualisation of the data produced in ever more imaginative and complex ways.

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From the Treasurer

BCA Bursary awards in 2000

During 2000, a total of £1520 was used for BCA General Bursaries. A donation of £500 was made to the Glasgow Protein Workshop to support student attendance. Bursaries totalling £4481.21 were awarded through the Heriot Watt Spring Meeting accounts. The administration of bursaries has been reviewed and new procedures implemented to speed up the decision making process and ensure that guidelines are followed.

19th European Crystallographic Meeting

Nancy, France 25th-31st August 2000

The ECA conference this year was held in the picturesque city of Nancy, capital of the Lorraine district of France. By day, we enjoyed the science, and on the warm evenings, we enjoyed a beer or two around the main square. This year saw new special interest groups in Extreme Conditions and Diffraction Physics. With the help of a BCA Bursary, I was able to travel to the conference and present my work on a poster entitled "Under Pressure: Hydroxylamine" in the Extreme Conditions: New Developments session. The poster showed the results of a high-pressure study on d3-hydroxylamine (W.G. Marshall, C.R. Pulham, P.A. McGregor, D.J. Francis, ISIS2000 Report for PEARL/HiPr Experiment RB10655).

The Extreme Conditions microsymposia began with a plenary lecture on "Structural Phase Transitions of Simple Metals under Pressure" given by Karl Syassen of the Max Planck Institute in Stuttgart. He gave an overview of the structural changes of the alkali metals under pressure. Potassium, rubidium and caesium undergo a *s* _ *d* transition, they essentially turn into monovalent *d* transition metals. As metals adopt complex crystal structures under pressure, angle dispersive synchrotron x-ray diffraction is required to gain sufficiently good data for structure solution.

Martin Kunz from Zurich delivered a very informative talk entitled "High Pressure powder crystallography using synchrotron and neutron radiation". In this, he gave an overview of the equipment used, including the Merril-Basset diamond-anvil cell for x-ray work and the Paris-Edinburgh high-pressure cell for neutron diffraction. The use of laser heating in the diamond–anvil cell increases the temperature range to several thousand Kelvin. This coupled with the megabar pressure range of the cell and synchrotron radiation, enables *in situ* experiments. The third generation synchrotron beam has a small, brilliant x-ray spot of 10 _m, which has a diameter less than that of the laser beam. This is excellent for the powder data collection at the above P-T range, although the conventional pressure measurement using pressure sensitive fluorescence lines is no longer reliable, and an equation of states measurement is required using an internal pressure standard.

On the penultimate afternoon, there was an excellent session on "Advances in Hydrogen Bond Research". The first talk was given by Gastone Gilli of the University of Ferrara in Italy, entitled "Hydrogen Bonding in the Last Quarter of the Century: New Methods, New Results, New Ideas". An overview of the research and development of the techniques involved and the results obtained over the past 25 years was given by addressing four key H-bond topics. These are the bond energies, the electrostaticity and covalency, the electronegativities and relative proton affinities, and the strong H-bond chemical leitmotifs.

There were also a number of oral presentations on intermolecular interactions, in particular a plenary given by Ingeborg Csöregh of Stockholm University who showed a range of crystal structures in which the halogen-halogen contacts were very short. In the Neutron Diffraction microsymposia, Chick Wilson of ISIS gave an entertaining overview of what is "State-of-the-art in Time-of-flight Neutron Diffraction".

Pam Mcgregor
Edinburgh University

IUCr International Workshop on Crystallography at High-Pressure and High-Temperature Using X-rays and Neutrons

Spring-8 Hyogo, Japan 30th Sept to 3rd Oct, 2000

The setting for the conference was the SPring-8 Synchrotron Source in Hyogo, Japan. Built at 1000ft above sea level on the flattened top of a mountain, SPring-8 (Super Photon ring 8Gev) is a source which rivals the ESRF in terms of stunning scenery. It also boasts the brilliance expected from the worlds most powerful third generation synchrotron source, and has a science programme to match. The impressive scale of the science was demonstrated on the first night by a tour of the synchrotron and the extensive array of high-pressure sample environment. All ninety attendees had travelled from around the globe as well as from Japan itself to attend this High-Pressure, High-Temperature Workshop. The programme was condensed into three days, and was packed with exciting new science in the field of extreme conditions. The sessions attended were Random Systems, Novel Structures of Simple Systems, Geophysics, Crystal Chemistry and Material Science. The topics covered spanned a huge range of crystallography, including phase transitions in liquid phosphorous, the synthesis of super-hard materials from C-60 and a lively debate on the high-pressure phase diagram of oxygen.

My own presentation was a poster describing recent development

work in the use of single-crystal techniques for neutron diffraction at high-pressure. In addition to the poster session, I was able to present my work in a five minute oral summary. This received a reasonable level of interest in its novel use of time-of-flight Laue diffraction for high-pressure work. I found it extremely beneficial to meet and interact with a group of people possessing such a broad range of technical expertise. This was perhaps the most important aspect of the conference for me - that is, the exchange of technical solutions to problems which I had encountered in my own research. In addition, immersion in the science of so many experts in the field of high-pressure science has certainly broadened my horizons as a young scientist. However, the conference was not all hard work. Devising a social programme in a location as isolated as SPring-8 presented the organisers with a certain challenge. This was a challenge that was met in a uniquely Japanese way: the Tatami Room. This small rectangular room with paper walls and low tables was where we met each other in a situation less formal than the lecture room. The traditional saké was served as well as (the slightly Less traditional) Japanese Brie! We were also treated to an exquisite conference banquet overflowing with sushi-me and a traditional Japanese tea ceremony. In summary, this meeting was extremely fruitful for me scientifically. This was a direct consequence of my interaction with scientists who are Experts in the field of high-pressure. In addition to this, the cultural aspects of a visit to Japan added a unique and memorable flavour to the meeting.

Malcolm Guthrie
University of Edinburgh

The Ninth International Conference on High Pressure Semiconductor Physics (HPSP IX)

The Ninth International Conference on High Pressure Semiconductor Physics (HPSP IX) was held in Sapporo this year, the capital of the beautiful Island of Hokkaido in the North of Japan. The meeting was spread over four days (four mornings and two afternoons). The scientific programme covered different areas in the field of semiconductor physics at high pressure, from the "Theory of the High Pressure Phases of IV and III-V Semiconductors", an excellent opening talk given by G. Ackland from Edinburgh University, to "Photo-Induced Structural Transformations of C60 Single Crystals under High Pressure" by T. Mitani from the University of Tsukuba.

I gave an oral presentation entitled "High-Pressure High-Temperature Structural Ordering in GaSb", the main subject of my PhD thesis, in the first afternoon session of the meeting, which generated a lot of interest. It was a fantastic opportunity for me to present, for the first time, the results of my experimental work to the international scientific community in my field of research and to exchange ideas with the world-expert theoreticians in high-pressure semiconductor physics. At the closing ceremony, I was awarded the Young Scientist HPSP IX award based on the scientific quality of the work. This award was presented to only a few students and postdocs at the meeting.

The social programme was very much focused on experiencing Japanese culture. Delegates were invited to a half-day excursion to the Noboribetsu Hot Spring followed by a Japanese-style banquet. Not neglecting to mention the fortunate delegates that arrived before the start of the conference, who had the opportunity to take part in a "kimono-wearing" session followed by the traditional tea ceremony. It is no doubt that this conference was a success at both the scientific and social level.

Two days after the HPSP IX Conference, I went to SPring-8 to attend the third International IUCr Workshop on "Crystallography at High Pressure and High Temperature using X-rays and Neutrons". The meeting started with the tea ceremony (another one!) followed by a get-together party in a very friendly atmosphere. The workshop was extremely well organised, with each day offering a variety of oral sessions which I found very rewarding (random systems, novel structures, geophysics, crystal chemistry, materials science, etc.).

At the end of the first day, a very interesting site tour of Spring-8 was organised, giving the delegates the opportunity to visit the various high-pressure beamlines of this world-leading facility. The site-tour was extremely interesting as it was my first visit to an overseas research facility and it is no doubt that, having performed my PhD experiments at SRS in Daresbury, this visit was greatly valuable as it provided me a wealth of information about recent high-pressure beamline technology developments. The second day featured a lively afternoon poster session, where I presented my work, followed by the workshop banquet, where the finest Japanese food and drink were served.

Despite the isolated location of SPring-8, various social activities were organised in the evenings: games, saké tasting and the "Spring-8 Olympics Arm Wrestling Competition" in the tatami room. Once again, the Japanese did not miss the chance to show their true hospitality and make this event an unforgettable experience for all the participants.

Miss Van Petegham
Edinburgh University

The Weirdest known struture of any element

article reprinted courtesy of
CLRC Daresbury Laboratory

At atmospheric pressure and room temperature almost all the metallic elements, such as copper, iron and magnesium, adopt simple high-symmetry crystal structures. However, applying pressure to these elements changes the electronic structure of their atoms and this can give rise to a sudden change in structure, or phase transition, to one that is much more complex. As the electronic structure of the atoms in high-pressure phases can be quite different to those found in an element at ambient pressure, they are effectively 'new' pressure-induced elements. High-pressure phases exist deep within the Earth and other planets where their centres are at very high pressure and temperature. This has important implications for our understanding of the chemistry and mineralogy of planetary interiors. In addition, the ability to make 'new' elements in the laboratory opens up the possibility to create a wide range of wholly new materials.

Barium (Ba) and strontium (Sr) are examples of elements that have simple cubic structures at ambient conditions. However, pressure-induced changes in their electronic energy levels result in very complex crystal structures that have resisted all attempts to obtain a satisfactory solution for the last 30 years or more. Recently, Professor Richard Nelmes, Dr Malcolm McMahon and colleagues from the Department of Physics and Astronomy at the University of Edinburgh have used powder and single-crystal diffraction techniques at the SRS to solve the puzzle in the case of barium. This work was complemented by experiments using conventional laboratory X-ray data. The result is the discovery of an entirely new type of elemental structure that was described in the scientific journal, Nature, as 'the weirdest known atomic structure of any pure element'.

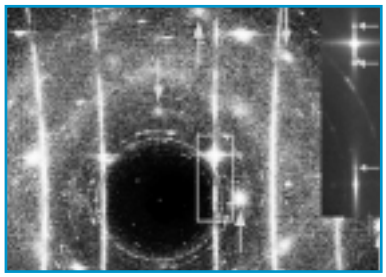

Figure 1
Figure 1 shows the diffraction pattern collected from a single crystal of Ba at 12 GPa (1GPa=109 pascals; or 10,000 times that of atmospheric pressure). The pattern contains four distinct components: sheets of diffuse scattering; single-crystal reflections lying on these diffuse lines; weak 'satellites' around these reflections (enlarged in the inset); and other single-crystal reflections which have a spacing different from that of the diffuse lines. These are marked by arrows.

The crystal structure that explains these features is shown in figure 2. First there is a body-centred tetragonal 'host' structure which gives the reflections in the lines marked by arrows in figure 1. This structure has channels running perpendicular to the page (the c-axis). Within the channels there are chains of atoms that form two different 'guest' structures. One is tetragonal and gives the strong reflections that lie on the sheets of diffuse scattering. The other is monoclinic and gives all the weaker 'satellite' reflections. The diffuse scattering itself arises from some positional disordering of the guest chains along the c-axis. What is most remarkable and completely unexpected is that the guest structures have a different spacing along the c-axis compared to the host and there is no distance over which the host and guest structures repeat themselves an integer number of times. The host and guest structures are thus said to be 'incommensurate' with each other.

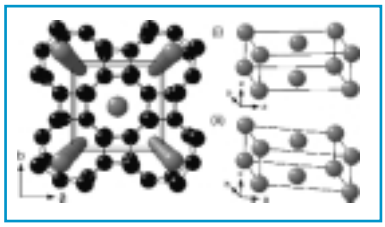

Figure 2.
The crystal structure of barium showing the body-centred tetragonal 'host'. Chains of atoms form the two different 'guest' structures.

This is completely new in an element. However, it has now been shown not to be unique to barium. Further work by the Edinburgh group at the SRS and also at the European synchrotron radiation facility (ESRF), Grenoble, has recently uncovered very similar incommensurate host-guest structures in strontium, bismuth and antimony. It is now a challenge to theoretical physicists to model this new structure type. Further work will almost certainly uncover other fascinating and new insights into metallic structures.

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Controlled release of drugs

article reprinted courtesy of CLRC Daresbury Laboratory

Over the past few years, pharmaceutical companies have been investing in the development of drug delivery devices, as well as in the drugs themselves. Many families of biodegradable polymers have been developed for use as drug release matrices. In such a system the drug is combined with the polymer, which is then implanted into the body. The drug diffuses out of the implant over a period of time, while the polymer matrix degrades harmlessly away. Some of these delivery devices are water-soluble and release the drug as the polymer matrix dissolves. Other polymer substances degrade more slowly in the body, such as polyglycolide - the polymer from which many degradable sutures are made. In this case, hydrolysis and erosion of the polymer controls the release of the drug.
For any drug delivery system, the release profile of the drug must be reliable and controlled. One major hurdle presented by this technique is that the diffusion process through a changing matrix is very complex. This means that it is often difficult to predict and control the release profiles of the drug molecules that are contained within the polymer matrix. Furthermore, incorporation of the drug itself may have an effect on the morphology of the polymer.

Using the SRS at CLRC Daresbury Laboratory, scientists from Cambridge University have been able to monitor the microstructural changes of quenched polyglycolide disks during degradation using wide-angle (WAXS) and small-angle (SAXS) X-ray scattering. Changes in crystallinity and lamellar structure were followed and these changes were then correlated with the observed drug release profiles.

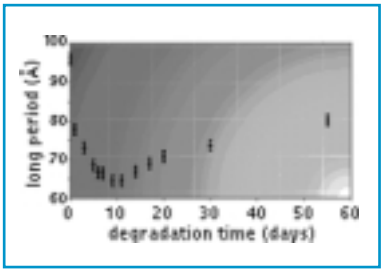

Figure 1: The long period of polyglycolide calculated by Bragg analysis of the Lorentz-corrected SAXS peak.

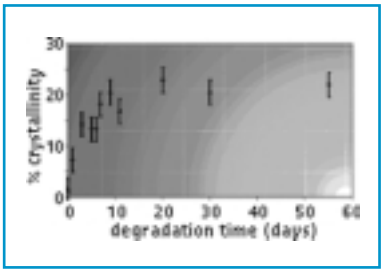

Figure 2: Changes in polyglycolide crystallinity during polymer degradation, calculated from the WAXS profiles.

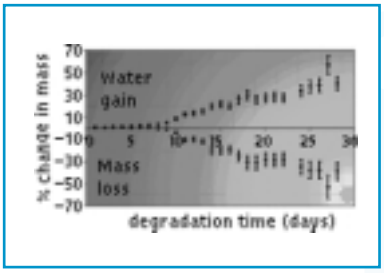

Figure 3: Loss of mass and uptake of water during polymer degradation, expressed as a percentage of the original mass of each sample.

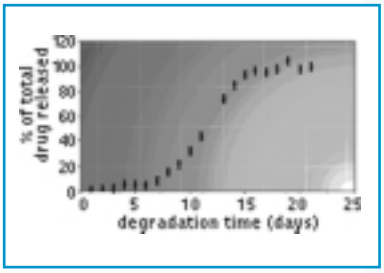

Figure 4: Release profile of the heat stable drug theophylline. Absorbances were measured using UV-visible absorbance spectroscopy.

The results in figures 1 to 4 show that at 10 days the degradation process changes: the long period reaches a minimum; the increase in crystallinity slows; there is a loss of mass and water uptake increases. It is at this point that drug release rate is at a maximum. The Cambridge scientists have now developed a model, based on these results and on previous work in this field. They propose that hydrolysis begins during the first 10 days, the molecular weight gradually decreases, insertion crystallisation causes the long period to fall and only a small amount of the drug can diffuse through the dense polymer matrix. However, at around 10 days the polymer reaches a critical molecular weight, and some of the oligomeric degradation products are able to diffuse out of the surface regions. This process creates spaces in the resulting semicrystalline structure which then become filled with water. Sharp reaction/erosion 'fronts' form between the dense polymer at the centre of the sample and the porous polymer on the surface. These fronts subsequently move into the centre, allowing the lamellar structure to swell and in doing so, drug and oligomers are released. Recent experiments using nuclear magnetic resonance (NMR) imaging techniques and nuclear reaction analysis have confirmed both the presence and the movement of these sharp reaction/erosion fronts.

Experiments have also been carried out to assess the impact of other variables on the degradation process; for example the thickness and initial morphology of the samples and the pH and concentration of the buffer solution. In every case the scientists have been able to correlate the morphological changes with the drug release profile. The further development of new and safer drug delivery systems is an important goal for pharmaceutical industries around the world. The ability to deliver a controlled dose over longer periods will undoubtedly improve current methods for the treatment of many chronic illnesses including cancer.

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Call for Proposals

Studsviv Neutron Research Laboratory (NFL)

EU funded access to Large Scale Facility Programme

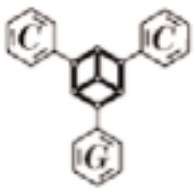
Since 1994 the DR3 reactor at Riso National Laboratory in Denmark and the R2 reactor at NFL in Sweden have operated a joint proposal system for their EU funded Access to Large Scale Facility programmes. However the recent decision to close the DR3 reactor means that the joint system can no longer be continued. The new NFL proposal system is very similar to the previous joint Riso/NFL system. Calls for proposals will be issued every four months (normally April 1, August 1, December 1) - however now there will be no deadlines for submission of proposals. Proposals should be submitted directly to NFL - not to Riso as before. Note that it is also possible to apply for training of new students, or training in new techniques. In this case the proposal does not have to be linked to a specific experiment - in some cases it is more effective to use a 'model' experiment for training purposes.

For powder and single crystal diffraction (NPD, SXD), residual stress and texture measurement (REST), you will find that the performance of the NFL instruments is very similar to that of the comparable Riso instruments. NFL can also offer the SLAD diffractometer for diffraction studies of disordered materials (liquids, glasses, disorder in crystals), the TTOF thermal time-of-flight spectrometer and the OSIRIS radioactive ion source/isotope separator. For more information on our facilities or the Large Scale Facility programme, please visit our web site at http://www.studsvik.uu.se.

from Rob McGreevy

Computational Tools in Chemical Crystallography

CCG Autumn Meeting Smithkline Beecham, Harlow



The Autumn meeting of the CCG, held on 15th November, was attended by 89 people. In addition to the scientific sessions, tours of SB's Discovery Chemistry facilities before and after the scientific sessions were available. The meeting began with a welcome from the local organizer (Roy Copley) and the head of SB's Medicinal Chemistry (Europe), Professor Peter Machin.

Jonathon Goodman (Cambridge) started the scientific session with his talk on "Understanding Molecules: Computational Approaches". He demonstrated a number of web-based tools (see http://www.ch.cam.ac.uk/magnus) for presenting the results of a number of different systems. After a brief introduction, he moved onto the practical application of computational tools to organic reaction mechanisms (particularly the isomerization of zaragozic acid). The relative proportion of isomers is predicted with increasing accuracy when more sophisticated models are used; the level of sophistication required for this to be useful is very high indeed. In another example, he showed that the stability and form of the hydrogen bonding patterns found when BH2F- Lewis acids co-ordinate to aldehydes can be explained by invoking an anomeric effect trans to the fluoride together with hydrogen bonding from the fluorine through the aldehyde hydrogen. He concluded by showing the results of energy minimization calculations on n-alkanes, and showed that, although short alkanes tend to adopt extended conformations, longer chains acquire stability through bends.
n-$C^{18}H^{38}$ has a bend at its global minimum, and a genetic algorithm shows that n-$C^{90}H^{182}$ folds into a 7 helix form. While the method has been extended to polypeptide chains, it is too early to predict protein folding via these methods.

Daniel Lynch (Coventry), made a "Request for Modelling Studies", and talked about some of the problems for molecular modellers that he has come across in molecular structures. He focused on adducts formed between phenoxyacetic acids and 2-aminopyridine derivatives. Crystal structures show that the phenoxyacetic acid fragment is found in both antiperiplanar and synclinal conformations, and molecular modelling studies show that they have roughly equal energies. In free ligands containing the 2-aminopyridine group, the N(1)-C(2) bind is 1.345(2)Å, and the amino N-C(2) bond is slightly longer at 1.351(1)Å. In adducts, the amino N-C(2) bond becomes shorter by some 0.03Å than the aromatic ring N-C bond. For the cases where 2-amino pyrazine is used for adduct formation, the same pattern persists. However, if the amino nitrogen has an alkyl group substituting a hydrogen, the expected bonding pattern is returned. He concluded by showing that similar patterns exist for other species and by remarking that current molecular modelling calculations do not predict these observations and as yet there is no real explanation for them.

Sally Price (UCL) talked about "Progress and Problems in the Computer Prediction of Organic Crystal Structures" and the reasons for and methods of predicting crystal structures prior to the synthesis of the target compound.

An electrostatic molecular model calculated in the gas phase followed by lattice energy minimization ignoring thermal effects (which gives rise to small errors in the cell lengths of around 3-6%). MOLPAK is used for the packing search. In some cases, e.g. 5-aza-uracil, the packing motifs predicted agree well with the crystal structure found experimentally. However, similar compounds such as 6-aza-uracil give rise to many predicted hydrogen bonded structures. While the experimentally determined structure is not the global minimum, it is very similar; when thermal libration is added to the model, the two become more or less indistinguishable.

The same conformer of paracetamol has two known polymorphs, $P2^1/c$ (form I, commercially important) and Pbca (form II, metastable). *Ab initio* modelling predicts these forms as the two lowest energy forms, but another polymorph (Form III) is unstable and only observed in melting experiments under a cover slip; of 12 structures predicted within 10kJ/mol of each other, any could be form III. Morphology predictions made on the basis of attachment energy improve the models (e.g. very slow growth in one direction results in "hard to grow" crystals). This information could be used to reduce the number of candidates for form III, bearing in mind the predictions do not include contributions from pressure.

Boris Shekunov (Bradford) took up the theme of using crystal growth energetics to explore "New Approaches in Prediction of Surface Energetics and Growth Anisotropy of Molecular Crystals". Working from known structures, several different aspects of crystal behaviour are used to calculate growth characteristics. He pointed out that although attachment energy theory states that the crystal shape is at equilibrium, and that growth rate is proportional to the surface energy of the crystal, the surface is not at equilibrium - steps on the surface are the most energetic parts of the crystal. In particular, he studied N-methylurea because different orientations of the crystal can be represented easily. Both numerical and Monte-Carlo methods were employed to investigate the relationships between the calculated parameters, supersaturation and the crystal morphology. He showed that not only can the shape of the growth step and the step velocity be predicted, but also that the crystal growth rate (giving the morphology) can be derived from a linear function, and this can be measured directly via laser interferometry.

Peter Bruce (St Andrew's) explained that "Challenging Structures solved from Powder Data", were tackled mainly for systems for which single crystals are not available, e.g most polymers. Powder data are limited when compared to single crystal measurements, for example peak overlap is a more serious problem, the peaks have an overall lower intensity, and there is inferior signal to noise ratio. Historically, the problem has been approached in reciprocal space, using methods adapted from single crystal methods, e.g. Patterson, Direct and Maximum entropy methods. As they all require considerable user intervention and hard work, they cannot be considered as routine. Rietveld analysis is a refinement technique and is not a method of structure solution. Direct space methods have been introduced more recently and include techniques based primarily on Simulated annealing (SA), Rudimentary Monte-Carlo methods, Genetic algorithms and adaptations of these using integrated intensities. The number of structural models generated by Monte Carlo methods is too large for all to be analysed thoroughly; a straightforward way to reduce it is to use rigid bodies and make use of chemical geometrical information. Even with a random model start, Rietveld Refinement cannot be used for structure solution as it uses LS and so can get stuck in false minima - LS is a "downhill only" process; simulated annealing is used to surmount this limitation. He continued by discussing difficult to solve structures, which usually fall into at least one of three categories, i.e. those with many degrees of freedom, those with more than one molecule in the asymmetric unit, and those which have heavy atoms in the AU along with flexible fragments formed by much lighter atoms. He finished with the example of PEO6 (polyethylene oxide hexamer):$LiAsF_6$; with 50 atoms in AU, and 79 variables including 15 torsion angles, it is the most complex powder structure solved to date.

Colin Seaton (Birmingham) continued the theme by describing "Investigating intermolecular contacts using POSSUM"; these help to explain the crystal packing, which in turn determines the bulk properties. Data from powders do not usually provide accurate enough geometric data for molecular structure solution. POSSUM uses a direct space iterated Monte-Carlo algorithm; solutions are evaluated, rejected or accepted according to pre-determined criteria and the process repeated until either a suitable result is gained or the scientist needs the computing resources for a more tractable problem. He demonstrated the ease of setting up a POSSUM structure solution job, and showed a number of examples of molecules solved by the program.

Bill Clegg (Newcastle) introduced Acta Crystallographica E; further details are in his BCA News article in December 2000. In a nutshell, Acta E will be taking over from Acta C electronic papers in order to provide rapid and efficient publication.

Guy Orpen (Bristol) described the importance of "Structural Systematics in Molecular Inorganic Chemistry". A new science is developing in the study of

collections of structures in the major databases. An obvious use is for obtaining typical molecular dimensions, and these can then be used in model building, both for validation and calibration.

The molecular flexibility in structures is apparent from data mining, e.g. Metal complexes are soft - M-L vary by 0.1 - 0.2Å, angles by 1 -2°, torsion angles by 10 - 20°. Clear correlations between dimensions have been determined in different types of compounds, e.g. C-P-C angles and P-C bond lengths in Transition metal phosphine complexes. In many cases the observations correlate well with calculations based on standard theories, e.g. VSEPR. Conformational variations can also be followed. Further, intramolecular bonding patterns become apparent when the CSD is studied.

Reaction pathways investigated via analysis of structure correlation include metal cluster rearrangements and halide exchange at Sb. However, the Potential Energy hypersurfaces calculated are not unique and have a non-Boltzmann distribution, so some caution must be employed.

Investigation of anecdotal evidence of some specific intermolecular interactions has shown that some do not occur, e.g. organochlorines do not hydrogen bond. "Supramolecular synthons" identified in the CSD have been used to influence the packing in the crystal structures of new compounds, and provide an analogy with hydrogen bonding.

The current prospects of further advances are bright; methods are developing quickly and the main source of data, the CSD is expected to double in size over the next ten years.

Harry Powell
CCG Secretary/Treasurer

Crystallography in Industry

Roche Discovery, Welwyn Garden City, 1 November 2000

Brett Cooper (Merck Sharp & Dohme) opened the meeting with a case study showing how powder diffraction, although not often the technique of choice, can be used as a quantitative tool for monitoring polymorphic conversion in both drug substance and product. He discussed the inherent problems of powder diffraction for this application, such as preferred orientation, and how this had been approached. He concluded with an insight into the thermodynamic relationship between the two forms, and evidence suggesting that the conversion arose from recrystallisation in the presence of water rather than a solid-state transition.

Progress in indexing powder diffraction patterns was presented by Robin Shirley (University of Surrey). This included an introduction to why indexing can be difficult and a comprehensive survey of the algorithms available and their relative strengths and weaknesses, and an update on the progress of Industrial CrysFire. He concluded with a demonstration of CrysFire.

Chris Frampton (Roche Pharmaceuticals) presented recent zopiclone results as an update to his presentation at the Spring Meeting. This included elucidation of the crystal structure of the anhydrous monoclinic form from synchrotron powder data, enabling comparison with the previously obtained single crystal structures of the monoclinic dihydrate and orthorhombic anhydrate. Comparison of the two monoclinic forms clearly demonstrated the dramatic changes that can result from ingress of water into channels in the structure. The changes in inversion symmetry for the anhydrous forms suggest that there may be a racemic to enantiomeric transition.

The BCA representative to ICDD, David Taylor, described the role of the ICDD and how its membership is made up. He then gave a report on recent developments within ICDD. These included the move away from paper products to a range of Relational Database CD-ROM's thus reducing costs, electronic purchasing, workshops and conferences, and new licences.

Following lunch, provided by Roche Discovery, the afternoon session opened with Dr Steve Norval who presented the Industrial Group Award to Dr David Dyson for his contribution to the field of X-ray diffraction. The Industrial Group Award Lecture which followed gave a fascinating insight into the life of a practitioner of X-ray diffraction over the years with an emphasis on the measurement of texture.

Steve Norval (ICI) then provided an update on the progress towards the release of an EU Standard covering X-ray diffraction. A standard is required as there is currently no National or International point of reference to encourage good practice, and to act as a point of reference. The General Principles section will be the first part to be released; possibly this year. Its release will impact on all uses of X-ray equipment working in a regulated arena.

Judith Shackleton (Manchester Materials Science Centre) provided a report on the Structural Materials Workshop held earlier in

the year. The workshop was seen as a big success in bringing together people who work in this field and covered the pros and cons of sample preparation techniques. Finishing, Judith made a request for ideas to be made for future meetings.

Dr Liz Town-Andrews (DARTS) reported on the workshop held in October to communicate their objectives to industry. Liz related that a lot had been done to make the facility much more accessible to industry and that they now able to offer a service based on a charge per sample or problem. An example of this service is afforded by station 9.8, which deals with micro diffraction. They will now, on the basis of no success no charge, attempt to solve the crystal structure from very small crystals (>20mm in all dimensions); the cost of success £4000.

Paul Tattersall (NRPB) gave an update on the impact of IRR-99 which became effective from 13th May 2000.

The legislation covers employers intending to use electrical equipment to produce X-rays for industrial radiography, processing of products, research and finally exposure of persons for medical treatment accelerators (except electron microscopes).
The regulation covers Prior Authorisation, Notification of Work, Prior Risk Assessment, Restriction of Exposure, Engineering Controls, Dose Limitations and Contingency Plans.

Philip Lake
Clare Anderton

Geometric symmetry in patterns and tilings
by Clare E. Horne

Publisher
Woodhead Publishing
23 October 2000 £95 US $157
***ISBN* 1 75573 492 3**
256 pages hardback size 215 x 303mm

Introductory text books of crystallography often contain a short chapter on the 17 plane groups but they rarely have space to go into detailed explanations and give illustrations of patterns of each type, before going on to the more complex three-dimensional space groups. This can leave some students unable to understand the subtleties of the more complex groups. This book could be an excellent reference work for a library where students of crystallography (or those studying it as part of courses in chemistry, materials science, earth sciences etc.) can study the two dimensional patterns in greater detail to become familiar with the symmetry and other operations involved in their production.

There are 6 chapters: Introduction, Classification of design by symmetry group, Classification of design by symmetry group and design unit, Classification of discrete patterns, Classification of isohedral tilings and Summary and conclusions. Each chapter has its own summary and list of references. The book has over 1000 illustrations of two dimensional patterns and includes simple instructions on how to create them. Most of the diagrams are original; they were made using the Harvard Graphics package, which the author found rather inflexible. On page 37 there is a useful flow diagram for symmetry group identification of ditranslational designs. It would be interesting to try this on the design based on a crystal structure as part of the 1951 Festival of Britain reprinted on page 22 of the last issue of *'Crystallography News'.*

The author is a mathematician who gained her PhD from the University of Leeds in the combined disciplines of mathematics and design. She thinks that good textile designers intuitively understand that their patterns are more satisfying if they obey the geometric symmetry and translation rules summarised in the 17 plane groups so she has written this book in an attempt to help *all designers* to improve their work by a better understanding of the geometry. She assumes that designers have no formal mathematical training and tries to explain from first principles how each plane group is formed by translation, rotation and reflection. The usual crystallographic notation is used for the groups and methods are given for the construction of designs based on each group.

The content of this book makes it an excellent teaching aid, particularly for those students with little mathematical training. Unfortunately, there are problems of poor layout on the page and in the reproduction of the figures, which I did not expect, in such an expensive book.

Kate Crennell
January 2001

Nanotechnology Mechanical and Electronic Systems on a Molecular Scale

Publisher
Institute of Physics
ISBN 07503 0749 8.

It is the first in a new series of Briefs designed to provide technical updates on current

applications of physics targeted at the non-specialist. This one is a useful description of the 'state-of-the art' in nanotechnology; a term which means different things to different people; this brief focuses on the manufacture of nanoscopic electronic and mechanical systems by molecular assembly. There is no attempt to cover making designer proteins or the wide use of nanotechnology in materials development, although the authors realise that perhaps some of the most promising lines of development come in areas which span these boundaries.There are plenty of illustrations and a page of 'Further reading' both in journals and on the Internet.

Two general references are:

The Institute of Nanotechnology
http://www.imm.ord/index.html
The Institute for Molecular Manufacturing
http://www.nano.org.uk

The one on **Nanotubes** at http://www.pa.msu.edu/cmp/csc/nanotube.html has links to Richard Smalley's home page where you can read his 1996 article *From Balls to Tubes to Ropes: New Materials from Carbon* a very readable account of the discovery of carbon nanotubes and their subsequent development.

This interesting booklet is available **free to members of the Institute of Physics** just send an email to **emma.woods@iop.org** quoting your membership number.
The price to non-members is £7.50. Order from Emma Woods, Institue of Physics, 76 Portland Place, London W1B 1NT

Kate Crennell
14 November 2000

Editors Note:
More articles and information about Nanotechnology is available in the
Annual Report 1999-2000
CLRC Daresbury Laboratory
at http://www.srs.dl.ac.uk/Annual_Reports/

for the 2001 ENSA/Walter Hälg Prize for European Neutron Scattering

The European Neutron Scattering Association (ENSA) are pleased to announce that the nominations for the second ENSA Walter Hälg Prize for European Neutron Scattering are now open. The detailed guidelines of the ENSA Walter Hälg Prize are listed on the ENSA web pages (www.psi.ch/ensa).

Nominations for the 2001 Walter Hälg Prize of the European Neutron Scattering Association (ENSA) may be submitted by European scientists as individuals or on behalf of a Division, Section or Group. To establish a high standard it is necessary that the Committee receive proposals that represent the breadth and strength of European neutron scattering. Nominations should include the motivation for the award, a brief curriculum vitae of the nominee and a short list of major publications. Letters of support from authorities in the field which outline the importance of the work would also be helpful. Nominations for the prize will be treated in confidence and although they will be acknowledged there will be no further communication. It should be further noted that all unsuccessful nominations for the 1999 Prize will receive automatic reconsideration for the 2001 Prize. Nominations should sent by post before 12 June 2001 to the Chairman of the Selection Committee:

Professor Bob Cywinski
Chairman of the European Neutron Scattering Association
Department of Physics and Astronomy
University of Leeds
Leeds LS2 9JT
UK

Forthcoming BCA meetings

Industrial Group

Pharmaceutical SIG meeting
7th June 2001, GlaxoSmithKline, Harlow

This one day meeting of the Pharmaceutical Special Interest Group will follow the well tried formats of previous meetings of the group by bringing together a range of speakers on subjects of topical interest. The programme information will be updated on the BCA web site as speakers and titles are confirmed. There is still space in the programme for contributions relevant to Industrial Crystallographers. For more information, or to offer a presentation of interest or please contact:

Dr C L Anderton
GlaxoSmithKline, New Frontiers Science Park (North),
Third Avenue, Harlow,
Essex CM19 5AW
Tel: 01279 627376
Fax: 01279 627374
Email: Clare_L_Anderton@gsk.com

Chemical Crystallography Group

Autumn Meeting
Mesomolecular Crystallography
Wednesday November 14, 2001
The CCG Autumn meeting 2001 will take place at Aston University on Wednesday November 14, 2001 and is entitled "Mesomolecular crystallography". It will focus on methods and experiences of structure solution, refinement and results for large small molecules. The local organiser is Carl Schwalbe (e-mail: c.h.schwalbe@aston.ac.uk).

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

PCG Rietveld refinement workshops

Introduction to the principles and practice of Rietveld refinement
17-18 October 2001 (provisionally)
Rutherford Appleton Laboratory, Oxfordshire

In Autumn 2001, the PCG will begin a series of tutorial workshops on powder diffraction profile refinement methods. This technique, much used and a vital component of much of physical crystallography, is very powerful but if improperly used can lead to problems both in the refinement process itself and in the resulting structural models. The aim of these workshops is to provide a general introduction to the method and its applications. They are aimed both at those new to the technique, particularly research students and post-docs, and those who feel the need for a refresher.The first of these workshops will be held in October 2001 at the Rutherford Appleton Laboratory, and will be two-day event introducing the basics of profile refinement using the Rietveld method. The workshop will include introductory lectures, demonstrations and hands-on examples. The local organisers will be Chick Wilson and Kevin Knight (RAL), with external input from Jeremy Cockcroft (Birkbeck) and others. Local overnight accommodation will be available. Full details including speakers will be announced on the Web site as they develop.
Contact Chick Wilson (C.C.Wilson@rl.ac.uk) for more details.

PCG Autumn Meeting

Applications of high pressure in structural studies
December 2001

The Autumn 2001 meeting of the PCG will be a one-day meeting covering the wide-ranging applications of high pressure techniques in the study of crystal structure, to be held in December 2001. Date and location to be finalised, but the meeting will include scientific presentations, brief accounts of the latest technical advances in pressure techniques for both X-ray and neutron diffraction, and a chance to view some of the advanced high pressure kit currently being made available on laboratory and central facility sources.More details will be available in the next issue of Crystallography News and on the PCG Website. For more information on the meeting contact the organiser:

Dr David Allan
(University of Edinburgh; dra@ph.ed.ac.uk) or the PCG **Secretary Chick Wilson** (C.C.Wilson@rl.ac.uk).

Summer School in Protein Crystallography

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

Summary of Forthcoming Meetings 2001

If you notice any errors or have news of any meetings to add to the Meetings List please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor, Jo Jutson, 4, Henlle Gardens, Gobowen, Oswestry, Shropshire, SYLL 3NU (more meetings listed on BCA website)

April 16 - 18, 2001
Accuracy in Powder Diffraction III, GAITHERSBURG, MD, USA
[e-mail: cline@credit.nist.gov]

May 23 - June 3, 2001
International Course in Crystallography, ERICE, Siciliy, 32nd Course:Strength from Weakness :
Structural Consequences of Weak Interactions in Molecules, Supermolecules and Crystals.[Details on the Web site or from Paola Spadon, Exec. Secretary, Int. School of Crystallography, Dept. Organic Chemistry, Via Marzolo 1, 35131 Padova, Italy; fax: +39 049 8275 239 email paola@chor.unipd.it]

June 7, 2001
BCA Industrial Group, Pharmaceutical SIG Meeting, GlaxoSmithKline, New Frontiers Science Park, Harlow[For further information contact:Dr C L Anderton, GlaxoSmithKline, New Frontiers Science Park (North), Third Avenue, Harlow, Essex CM19 5AW Tel: 01279 627376 Fax: 01279 627374 Email: Clare_L_Anderton@gsk.com]

June 13 - 15, 2001
10th Annual Meeting of the DL CCP on Fibre and Non-Crystalline Diffraction, STIRLING, Scotland [arranged by CCP13 details will be posted at http://www.dl.ac.uk/SRS/CCP13 as soon as they are available]

Summary of Forthcoming Meetings 2001 cont.

June 21 - 24, 2001
10th Croatian-Slovenian Crystallographic Meeting Lovran, Croatia, Website http://www.chem.pmf.hr /~hkz/lovran01/ [Details from Stanko POPOVIC spopovic@phy.hr, Phone: ++385-1-4605-549, Fax: ++385-1-4680-336]

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

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

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

July 30 - August 3, 2001
Denver X-Ray Conference, STEAMBOAT SPRINGS, CO, USA [Advance information indicates special emphasis on SAS methods, especially in polymers, details at http://www.dxcicdd.com/]

August 1 - August 3, 2001-01-22
Neutron and Hard X-ray Optics and Applications, San Diego, CA, USA [Further information from IUCr Web site]

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

Corporate Members

Bede Scientific Instruments Ltd

Cambridge Crystallographic Data Centre

Hampton Research

International Centre for Diffraction Data

Molecular Structure Corporation

Oxford Cryosystems

Philips Analytical

BCA Corporate Membership

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

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

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

The cost of this membership is £600.00 per annum

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

BCA Administrative Office
Northern Networking Ltd
Bellway House
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Glasgow
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Phone 0141 954 4441
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e-mail BCA@glasconf.demon.co.uk