BCA IG Newsletter

February 2005

EDITORIAL

Welcome to this latest issue of the IG newsletter. There are a number of excellent meeting reports in this issue along with details of the forthcoming Spring Meeting and two-day Autumn Meeting. Please do try to come along. At the AGM, proposed changes to the Industrial Group Constitution will be discussed concerning membership of the Committee and their nomination. Please read the Chairman's thoughts on this very important matter on page 2. Please also read the proposed changes on the same page and contact the Secretary/Treasurer if there are issues you want to raise concerned with these changes. The AGM is on Wednesday 13th April at 4pm. Please make every effort to attend.

The Committee is proposing a two-day Autumn meeting again this year with themes around Patents and Crystallography in Industry. Make a note in your diary now.

Finally, a big thank you to all those who have written contributions for this issue.

Phil Holdway

WE NEED YOUE HELP! PLEASE PASS ON THE ENCLOSED XRF MEETING INFORMATION TO YOUR XRF COLLEAGUES OR ANYONE YOU KNOW WHO MIGHT BE INTERESTED!

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Forthcoming Events 2005

Registration available on the WEB.

BCA Spring Meeting 2005.

Loughborough University, 12-14 April 2005

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Autumn Meeting 2005

Birkbeck College , London, Oct 18th – 19th

Oct 18th – Workshop on Patents in Crystallography

Oct 19th – Patents and Crystallography in Industry

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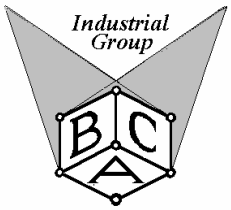
Further details in the next issue.



Charity Registration Number: 284718

World Wide Web addresses:
BCA http://www.crystallography.org.uk
IG http://www.crystallography.org.uk/ig/ig.htm

THANK YOU

Thanks to **Hiltonbrooks** **'celebrating 25 years'** for sponsoring the cost of production and distribution of this edition of the Industrial Group Newsletter.

www.xrays.u-net.com

FROM THE CHAIRMAN:

This issue of the BCA Industrial Group Newsletter will bring to your attention a proposed change to the constitution rules of the group. Although I find it sad to see more and more industries abandon the use of their own research laboratories in favour of out-sourcing to other laboratories, particularly those in academia, nonetheless one has to recognise the facts. It has been particularly noticeable in the last six months as several committee members have found themselves at the heart of laboratory closures. Although I still perceive the BCA Industrial Group to be in healthy state, I feel it is important for our future that the number of committee members from academic institutions is no longer limited to three as in the present constitution. For this reason, proposed changes to the constitution are being made to the membership for discussion and hopefully your approval at the next AGM.

Personally, I feel that the program for the next BCA Spring Meeting should be suited to those with an interest in industrial crystallography given the themes of in-situ and non-ambient crystallography as the majority of industrial processes are carried out under a variety of conditions. As a member of this year's programme committee, I conveyed the ideas of the BCA-IG committee so as to provide a variety of programme slots in this year's Spring Meeting of interest to BCA-IG members. In addition, through the hard work of two of your committee members, Dave Taylor and David Beveridge, there will be a parallel programme on the subject of XRF, a first for a BCA spring meeting. At the present moment, XRF being an X-ray spectroscopic rather than a diffraction-based technique has no home within the BCA. So a further subject for discussion at this year's AGM will be whether the Industrial Group should consider enlarging its membership base beyond its traditional strength in PXRD so as to include XRF. Obviously, this would require further changes to the constitution, but I look forward to a lively discussion on this subject, either at the AGM or by email to me if you cannot attend.

The past 6 months has been busy for your chairman too. Although our old *Industrial Materials Group* laboratories at Birkbeck are being demolished to make way for biophysics group in the School of Crystallography, Paul Barnes and myself have moved on to newly-built laboratory space within the new *Materials Chemistry Centre* within the Department of Chemistry, UCL. But while we are the fortunate ones with a bright future ahead, I still empathise strongly with those less fortunate and under threat of laboratory closure. Despite these problems for some, I do hope that most of you will still have the opportunity to attend this year's meeting and AGM at Loughborough,

Jeremy Karl Cockcroft (Chemistry, UCL &
Crystallography, BBK).

Industrial Group AGM

The 22nd ANNUAL GENERAL MEETING of the Industrial Group will be held at Loughborough at 16:00 on 13thApril 2004
Nominations are sought to fill a vacancy for **one** committee member to serve for three years from April 2005.
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.

Proposed changes to BCA Industrial Group Constitution for the 2005 AGM

See the Industrial Group Website for full details of the Group Constitution

Introduction:

There is an ever increasing trend for Industrial Crystallography to be carried out in collaboration with Academic Institutions. In recognition of this fact, and as suggested by the membership at the last AGM, the committee of the Industrial Group proposes to change the wording of rules 11 and 15 of the BCA Industrial Group Constitution as follows:
Note the proposed changes are identified by: ~~deletion~~ and addition

11 COMMITTEE. The affairs of the Group shall be managed by a Committee consisting of the Officers of the Group together with no more than six Ordinary Members of Committee. ~~Not more than three Officers or Members of the Committee shall be from Academic Institutions.~~ The BCA representative to the ICDD shall be a member of the committee ex officio. Additional members may be co-opted from time to time under Rule 13. The Committee shall be broadly based, with no one field or discipline unduly favoured. Only members of the Group shall be eligible for Membership of the committee.

15 NOMINATIONS FOR OFFICERS AND COMMITTEE. Vacancies for Officers and Ordinary Members of the Committee shall be filled by election at the Annual General Meeting of the Group. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by (a) a brief statement demonstrating the nominee's experience in the application of crystallography to industrial research; and (b) 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.
These proposed changes will be put to the membership for discussion and approval at the next AGM to be held at the BCA 2005 Spring Meeting in Loughborough.
Contact the Secretary/Treasurer if you have any comments

Introduction to Powder Diffraction – One Day Workshop

Manchester Materials Science Centre, 10th June 2004

This event was hosted by Judith Shackleton and was aimed at people new to powder diffraction, those with some experience who need a refresher course or those considering the purchase of equipment. Our contingent from Liverpool John Moores University fitted that description perfectly. There were three of us in the party: myself, an academic with some experience of PXRD; a technician who has considerable experience; and a PhD student with none. We have recently purchased a new instrument and were appreciative of the opportunity to receive some training by the expert speakers at this meeting.

The venue was cosy, a seminar room in the Manchester Materials Science Centre. After being welcomed by Judith Shackleton, the first session was an Introduction to Powder Diffraction led by Jeremy Cockcroft. He outlined the differences between single crystal and powder diffraction and gave an overview of the factors that dictate the positions and intensities of peaks on a PXRD pattern.

Judith then discussed instrumentation and sample preparation and gave valuable insights into the operation and maintenance of a powder diffractometer. I had no idea that X-ray tubes lose intensity over time and have to be regularly checked and eventually replaced. She also talked about the importance of good sample preparation and how to overcome the difficulty of small quantities of sample. This was one of the most interesting and useful sessions for me and the smell of the awaiting lunch did not detract from the speaker.

After the buffet lunch, Dave Taylor spoke about the ICDD powder diffraction file and how this came to be the standard way of recording powder diffraction data. He related the history of the system and how it has arrived at its present form and the products currently available.

Jeremy Cockcroft took the floor for a second time to explain how powder diffraction can be used in quantitative analysis. He used a whole range of case studies from minerals to pharmaceuticals to illustrate how the different methods can be applied. For those with some knowledge of structural crystallography, the Reitveld method of refinement of data was discussed.

Judith Shackleton led the final session, which explored the use of other diffraction techniques including neutron and synchrotron techniques and residual stress measurement.

The day included several plenary sessions when the audience could pose questions to the panel of speakers, related either to the material covered or to problems encountered elsewhere. This was one of the most useful aspects of the day with many attendees asking questions and all of the speakers contributing to the answers. These sessions were often extended beyond the allotted time and even sent Judith off to the basement, returning with examples of equipment and sample holders to show the audience.

This workshop was extremely accessible in terms of duration and fee. Long training courses are hard to make time for and finding funds can be difficult. The geography, duration and low cost of this workshop meant that a contingent of three rather than a single representative was able to attend and as a result we were able to consolidate our understanding by discussions after the event. This was a very successful day, which should become a regular entry in the BCA calendar.

Linda Seton

School of Pharmacy and Chemistry

Liverpool John Moores University

Report on BCA Industrial Group - Pharmaceutical SIG Meeting on 5th October 2004.

This meeting of the Pharmaceutical Special Interest Group was superbly organised by **Anne Kavanagh** (AstraZeneca) and **Roy Copley** (GSK), and hosted by AstraZeneca at the company's picturesque Alderley Park site.

After a warm welcome to the meeting by Anne, **Rebecca Booth** (AstraZeneca) explained the importance of hydrate formation in the development of new drugs and the strategies available for screening compounds for hydrate formation. Whilst vapour sorption studies are very valuable for studying hydration processes that are governed by fast kinetics, they are not so useful for investigation of hydration processes that are under thermodynamic control and for which the kinetics may be slow. Such systems are best studied using a slurry method that relies on the activity of water being directly related to relative humidity. Rebecca illustrated the advantages of the slurry method using two case studies, theophylline and an AZ compound. For both cases, the slurry method proved much faster at assessing the relative stabilities of hydrates and anhydrous forms.

Chris Hunter (University of Sheffield) then explained how 1H NMR methods can be used to study crystal nucleation in solution. The technique was originally developed to obtain structural information from the changes in chemical shift caused by complexation between two components to form a weakly bound complex. Chris explained how the technique can be extended to obtain structural information about molecular aggregates during the initial stages of precipitation. Chemical shifts are calculated *ab initio* for small molecules and then these are applied to larger molecules. A genetic algorithm approach is used to refine the chemical shifts allowing the structural model to be optimised by comparison of calculated and observed chemical shifts. The technique was illustrated with sulfamerazine, for which the solution-phase aggregate matches very closely the X-ray crystal structure, and carbamazepine for which the solution-phase structure is solvent dependent. In general, the method works well for relatively rigid molecules and for those for which there is an abundance of chemical shift information.

After coffee, **Gareth Lewis** (AstraZeneca) introduced the importance of salt selection studies in order to optimise the physicochemical properties of a drug. Interestingly even taste can be an important factor, especially for paediatric medicines. Gareth illustrated how remacemide, a potential antagonist for epilepsy, Parkinsonism and Huntington's disease, was crystallised as a variety of salts that were subsequently investigated by X-ray diffraction. The crystal structures clearly showed hydrophobic and/or hydrophilic regions depending on the nature of the counter-anion. The hydrogen-bond motifs were also analysed. Interestingly, the size and shape of the anions appeared to have very little effect on the types of structure observed.

Ed Collier (formerly UMIST, but now The University of Manchester) continued with the theme of salt selection and described the work performed during his PhD. This involved the preparation of a further 23 salts of the pharmaceutical compound (1R, 2S)-(-)-ephedrine using combinatorial techniques. Ed highlighted that during these crystallisation studies, several of the acids showed variations in their apparent acidity that depended on the solvent. From these salts, 19 crystal structures were obtained and the hydrogen-bonding networks and structure-property relationships were analysed. In addition to hydrogen-bonded motifs it is clear that -stacking interactions play an important role in many of the structures. The work has provided a starting point for a salt screening strategy and has improved understanding of the reasons for success and failure of commonly used anions to provide stable, crystalline salts.

After an excellent lunch and photo opportunity, **Chris Gilmore** (University of Glasgow) kicked off the afternoon with a presentation about how to identify polymorphs from the results of high-throughput screens that involve computer-controlled crystallisation and data-collection methods. Such data are frequently complicated by the presence of mixed phases, broad diffraction peaks, and preferred orientation. Chris explained how his program PolySNAP can be used to circumvent these problems. The technique relies on point-by-point matching of

powder patterns rather than simply by matching peaks. A combination of non-parametric (Spearman) and parametric (Pearson) statistical methods are used to obtain a correlation matrix. This is then used to generate a distance matrix, which acts as a source of classification to generate dendrograms, multidimensional metric scaling, silhouettes, fuzzy clusters and minimum spanning trees. These tools allow the data to be partitioned into clusters of related patterns. The program is very powerful and can readily detect mixtures of phases or components. Chris and his team have extended the technique to include additional data from Raman, infrared, and DSC measurements.

Doug Minick (GSK, North Carolina) then described the chiro-optical technique, of vibrational circular dichroism (VCD) to aid in the assignment of absolute configurations of chiral drug molecules. In VCD, polarised infrared spectra are first recorded for a compound in solution. Because of the time-scale of the infrared technique, contributions from all of the conformers present contribute to the observed spectra. Molecular mechanics calculations are therefore used to identify possible conformers and then *ab initio* calculations are then used to obtain the relative proportions of conformers present and most importantly the contribution each one makes to the VCD infrared spectra. After correction of gas-phase frequencies to solution-phase frequencies, the experimental and theoretical VCD spectra are compared and conclusions can be drawn about the absolute configuration of the chiral compound. Although the technique has some limitations, Doug currently reported a 96% success rate and he has had 15 assignments subsequently confirmed by X-ray diffraction.

Colin Pulham (University of Edinburgh) finished off the day with a presentation about the use of high pressure as a means of searching for new polymorphs and solvates. Although high pressure is widely recognised in the Physics and Geosciences communities as a powerful means of inducing phase changes, it is not a technique that has been widely explored by the chemical or pharmaceutical communities. Colin illustrated how recrystallisation in diamond anvil cells can be used to prepare and characterise new polymorphs and solvates of phenanthrene, paracetamol, and piracetam. These experiments can be scaled up and in some cases bulk quantities of these polymorphs and solvates can be recovered to ambient pressure. He also demonstrated how the technique can be used to screen for polymorphs by showing that the 3 known forms of piracetam plus a new form can be selectively recrystallised simply by changing the pressure.

Roy Copley concluded the day's proceedings by thanking the speakers and participants, and urged everyone to support the Spring BCA Meeting that will include two sessions on the subject of non-ambient pharmaceutical studies.

Colin Pulham
University of Edinburgh

Industrial Group E-mail Mailing list – Online registration.

The IG sends about six E-mail notices each year to anyone interested (You don't even need to be a BCA member!). These inform of Newsletter postings and the various meetings we organise each year. You can now register for our E-mail list online - follow the link from the IG home page. There is an opportunity to be removed from the list with each mailing.

SPONSORS WANTED

The Industrial Group is always looking for new sponsors for this newsletter.

Potential sponsors, whether individuals or companies, should contact the editor or any member of the Industrial Group Committee for further information.

Sponsors will have an acknowledgement on the front page of both the paper and web newsletters and if relevant, a company logo and web address.

BOOK REVIEW: "X-Ray and Electron Diffraction Studies in Materials Science"

Author: D J Dyson *Publisher:* **Maney** 2004 368 pages
Price: (hardback) £78 ($133) ISBN 1902653742

It is good to see a new book on x-ray and electron diffraction aimed at the less experienced analyst working in a materials laboratory that will also find use as an undergraduate learning aid. Supplying the units in formulae throughout the text is welcomed and will assist more detailed calculations. The author draws on his 40 years experience in the steel industry to add a wealth of real examples to illustrate the subject. The text covers a wide range of topics including useful sections on texture and electron diffraction which add to a balanced overview of the subject and its everyday application to Phase ID, quantitative and size strain analysis. The book is well supported with photographs and clear diagrams which complement the text as do comprehensive references.

The first half of the book has sections on; real space, crystal chemistry, intensity of diffraction, stereographic projection, instrument consideration and line profiles which provide a good grounding in the basics of crystallography and the theory of diffraction. The first chapter (p1 - 44) on Real Space gives a very clear introduction, through; symmetry, lattices, space groups to Bragg's law, of the basic crystallographic concepts needed for a full understanding of diffraction.

The second chapter (p45 - 76) on Crystal Chemistry encompasses the packing of atoms within the crystal structure, building up from simple to complex inorganic systems and covering interstitial phases, metallic glasses and silicates. The next chapter on Intensity of Diffraction (p77-98) covers the factors which influence the intensity of a reflection and the equations needed to calculate its intensity, focussing particularly on the cubic system. The fourth chapter provides a useful explanation of Stereographic Projection (p99 -114) underpinning its use in later chapters. The next chapter on Instrument Considerations (p115 - 135) covers just the basics for x-ray diffraction and offers simple practical information on instrument parameters. The sixth chapter is devoted to Line Profiles (p136 – 160) and explains the factors which affect the size and shape of diffraction peaks and offers useful advice on the use of peak fitting routines.

Chapter 7 sees a move into applications and covers Phase Identification (p161 - 189). It starts with peak location and associated errors, moves on to intensity and then identification. It has sections on precision, reference materials and the figures of merit used to scale database searches. The next chapter covers Quantitative Analysis (p191 - 234) and starts with validation which is becoming increasingly important as we strive for standardisation. It covers sampling and preparation, instrument considerations specific to quantitative work and the various procedural methods. Particular cases are studied including: airborne dusts, glassy phase, metals and clay minerals. This chapter is supported by 44 references, more than any other. Chapter 9 covers Crystallite Size Analysis (p235 - 248) and offers practical advice on the various methods and their application. The next chapter covers the specialised field of Thin Layers (p249 - 271) and introduces the use of high resolution equipment and is followed by Crystallographic Texture (p273 - 317) which is well supported with useful pictures and diagrams which help put across what is often a difficult subject in a comprehensible way. A section on Electron Backscatter leads on to the final chapter on Electron Diffraction and its Relation to XRD (p319 - 354). Here theoretical aspects including the reciprocal lattice are interspersed with practical explanations and comparisons to provide a useful grounding in understanding the complementary nature of the two disciplines.

All laboratories working on the everyday applications of x-ray and electron diffraction will find this book a useful addition to their bookshelf.

Dave Taylor – December 2004.

Autumn Meeting "DIY Crystallography" 4th Nov 2004

School of Crystallography, Birkbeck College, London.

Forty delegates from UK Universities, Commercial and Industrial institutions attended this one-day meeting, organised by the Industrial Group of the British Crystallographic Association (BCA). The meeting was organised into two main sections - Hardware and Software. The speakers addressed the Do-It-Yourself aspects of crystallography which are widespread in the field due to the specialised nature of many activities which are not easily catered for in commercial instruments and software.

Building a High-Resolution Powder Diffractometer (Chiu Tang, DIAMOND) The synchrotron will have a 'medium' electron beam energy of 3.0GeV. The storage ring has a diameter of 561.6M and it has more than 20 bending magnets. Chiu showed a number of photographs obtained by a colleague flying a model helicopter containing a camera over the site! With 3 diffraction circles its design is highly versatile. The sample chamber is large (40x40x40 cm3) and there is a high precision, heavy-duty, xyz table.

Oscillating a sample for in-situ furnace studies (Olivier Leynaud, Birkbeck College, UCL) The project is focussed on in-situ experiments using gasses or vacuum at high temperatures. The furnace needs to be able to heat up to 950C and needs to accommodate capillaries with diameters up to 2mm. Different types of oscillating systems were investigated to oscillate, backwards and forwards, capillaries in the furnace: polarity, piston, wheel-like and it was the latter that was selected. Olivier showed some photographs of the completed device. The device oscillates at 68rpm with a 12V battery.

Industrial Polymer Processing Studies using Combined SAXS/WAXS Techniques (Ellen Heeley, Polymer Centre, University of Sheffield). Ellen began by saying that there is extensive use of polymer films in packaging. Texture is developed during processing but the nucleation in crystallisation is still largely a mystery. Ellen can record Small Angle X-ray Scattering (SAXS) and Wide-Angle X-ray Scattering (WAXS) data at the same time, which can be combined with rheology studies. The main areas for research are quiescent (slow processes) and sheer induced crystallisation / orientation.

Multiple Sample Holders (Mark Farnworth, Pilkingtonplc).
Mark described two multi-sample holders for the PANalytical Materials Research Diffractometer that he had designed and then had fabricated out of aluminium plate. Use is made of the batch programming software in X'Pert Data Collector. Sample x, y, and z values and the name of the data acquisition program are entered into the 'batch' program. Z values for each sample are determined in the conventional manner, using the dial contact gauge. Mark explained that the plate dimensions had to be carefully calculated to avoid contact with the primary optics and the sample stage.

A Multi-Sample X-ray Diffractometer with Photographic and Counter Recording (Jamie Nelson, Gemmological Instruments). Jamie described the work that he had carried out on the Debye-Scherrer photographic camera. His passion for tinkering with the camera, attaching items such as proportional counters, eventually led to him to receive Fellowship of the Institute of Physics. Jamie described several aspects of diffractometry hardware and used, for a relatively younger audience, unfamiliar terms such as Hole, Slot and Plane mounting or the 'Kelvin Mount'.

MATLAB: A Software Tool for Quick Data Analysis (Christopher Hall, University of Edinburgh). Christopher described his use of MATLAB 7. He finds several features particularly useful. These include good data input/output, built in utilities and functions, scripting (the stitching together of MATLAB commands into small programs) and a good graphic environment for reports and producing a common 'house' style. Christopher has built up a collection of scripts and utilities for handling synchrotron diffraction data - called XMAT.

Sharing Software Toolkits (By Ron Ghosh, ILL). Ron explained that over the last thirty to forty years there have been numerous computer languages from 'Plot 10' in the 1960's to modern day 'Windows'. Many of the packages have individual scripting languages and so this, and other complications, often deter the 'novice' from getting involved. He gave a simple demonstration of the use of Fortran for data display, plotting and filtering routines. Individual peaks can be selected for analysis e.g. line broadening. Ron finished the presentation by giving a number of useful internet links (see web version of report).

DIY Single Crystal Structure Analysis (Richard Cooper, University of Oxford)

Autumn Meeting "DIY Crystallography" 4th Nov 2004

Continued from previous page

Richard described the use of the 'Crystals' package for the analysis of single and twinned X-ray/Neutron Diffraction data. There are three main areas, Guidance, Validation Criteria and Tools. The Guidance step covers data collection (initial hkl analyses), early refinement, getting a complete model, later refinement, weightings and publication. The script language can access any crystal data or results. The Cambridge Structural Database (CSD) can be used to validate chemical geometry.

CCP14 Developments (Richard Stephenson, UCL, Birkbeck College).
The CCP14 website at www.ccp14.ac.uk contains freely available software, including state of the art algorithms and utilities. There is a concentration on crystallography. User feedback optimises the direction of the project. CCP14 contains multiple single crystal suites and multiple powder indexing programs and suites. It has 60GB of software and help files and has 35,000 monthly hits. It has a 'wiki' component (!) by which users can add comments that can be edited by any other user. Thus, the quality of the data is continually refined and improved.

Making do without the JCPDS (David Beveridge, Ilford).
David gave a series of steps that could be used to identify a diffraction pattern without the use of the JCPDS database. A good prior understanding of the sample would be ideal since this could drastically reduce the number of options for identification. A local library of patterns from reference materials can then be used for the search. A good understanding of the crystalline components in common materials would also be helpful. For example, paints contain rutile and anatase titania, kettle fur, soil and building dust contain calcium carbonate (calcite) whereas plaster contains hydrated calcium sulphate (gypsum).

CRYSFIRE Update (Robin Shirley, University of Surrey)
Indexing a powder pattern may only be a 6-parameter problem, but can still be a challenge. While methods of treating data have improved greatly, there is still great reliance on high data quality. Robin described the new CRYSFIRE now includes ten indexing programs with different approaches, and gives figures of merit for 10 or more indexing patterns. The newest version works with Windows XP.

Mark Farnworth
Pilkington European Technical Centre

Articles Wanted:

Why not put pen to paper and write a short article for our next Newsletter. There are lots of examples to give you some ideas in our Hints & Tips section on the WEB. Don't forget, if you attend a conference, please send in an article about it.

We are also looking to expand the range of Industrial Applications of XRD on our WEB Site. All we need are a few well-chosen pictures and a few words. How about something on CEMENTS, MINERALS, MUSEUMS, PHOTOGRAPHY, DETERGENTS, PIGMENTS, POLYMERS

INDUSTRIAL GROUP AWARD

It is the intention of the BCA Industrial group to make an Industrial Crystallography Award to suitable UK crystallographers working in industry or in academic institutions. The Award will be given in recognition of a sustained contribution to industrial crystallography including crystallographic and diffraction work of all kinds.
The Committee of the Industrial group will make the final decision concerning the Industrial crystallography Award. They intend the Award to take a form that fittingly marks the contribution made by the recipient.
Nominations for this Award are invited now and should be sent to the Secretary of the Industrial group. Besides the name and affiliation of the person proposed, nominations should state briefly why she or he merits the Award, giving a brief account (ideally not more than one sheet of A4) of her or his crystallographic work and its industrial significance. If desired, the proposer may suggest the form that the award should take.

BCA Spring Meeting 2005.

Loughborough University, 12-14 April 2005

There is considerable overlap with the Groups at this meeting and it important that you review the full programme on the BCA meeting pages. We concentrate here on items of particular interest to the Industrial Group.

NOTE: Day registration is only **£65** if you book early and 3 days fully inclusive of registration, meals, two nights basic accommodation and conference dinner is less than **£ 240**. Fully inclusive rates are available for less than **£155** for students and **£200** other concessions.

Industrial Group Highlights

There is something to keep you occupied over the full three days including a comprehensive exhibition featuring all the major suppliers, a real chance to update your product knowledge in a fast changing market place.

There will be a BCA Prize Lecture, Posters and Exhibition Open Evening with buffet & wine (18:30 - 22:00) on Tuesday 12th April see BCA Web pages for details.

2005 Spring Meeting Industrial Diffraction Highlights			
	Tuesday 12 April	**Wednesday 13 April**	**Thursday 14 April**
AM	**Registration & Exhibition**	**In situ Drug Discovery.**	**Non-ambient Pharmaceutical Studies 1.**
Coffee & Exhibition			
AM	**Plenary Session**	**In situ Diffraction Processing in Industry**	**Non-ambient Pharmaceutical Studies 2.**
Lunch & Exhibition			
PM	XRD,XRF and in-situ investigations on cementious materials. Herbert Pöllmann, Halle Univ.	**Crystallography in Industry 1.**	**Combined XRF/XRD Applications**
Tea & Exhibition			
PM	**Exhibitors talks**	**Crystallography in Industry 2.** **16:00 IG AGM**	
		18:30 BCA Prize Lecture	
Evening	**18:30 Posters & Exhibition 19:00 Buffet & Wine Reception**	**19:30 Conference Dinner**	

Exhibitors include:

Analysco, Beevers Miniature Models, BrukerAXS, Fluidigm, Genomic Solutions, Hiltonbrooks, Horiba Jobin Yvon, ICDD, Marresearch, Molecular Dimensions, Oxford Cryosystems, Oxford Diffraction, PANalytical, Perkinelmer Las, Rigaku, Spectro, Spex Certiprep

BCA Spring Meeting 2005 - continued

In Situ: Processing in Industry

Organisers: Jeremy Cockcroft & Steve Norval
Wednesday 08:30 - 10:00
08:30 Prof. Gordon Tiddy (Chem.Eng., Manchester)
Title TBA (Theme: surfactant formulation)
09:05 Dr. Geoff Moggridge (Chem.Eng., Cambridge)
"Processing block co-polymers for nano-pores"
09:40 Dr Simon Jacques (Chemistry, UCL)
"In Situ Crystallisation Studies of Pharmaceutical Materials"

Crystallography in Industry 1: 13:00 - 14:30 13th April 2005

Chair: Judith Shackleton, **Manchester Material Science Centre.**
13:00 Michael Preus, (School of Materials, University of Manchester.)
"Residual Stresses in Friction Welded Aeroengine Components"
13:30 Tony Fry, (NPL)
"Residual Stress Measurement at NPL, Increasing Confidence and Developing Best Practice"
14:00 Martijn Fransen, (PANalytical)
"To be advised"

Crystallography in Industry 2: 15:00 - 16:00 13th April 2005

Organisers: Richard Morris & Martin Gill
15:00 Peter Laggner, Institute of Biophysics and X-Ray Structure Research Austrian Academy of Sciences.
"Bridging the Nano-Gap: Simultaneous SAXS and XPD on Nanomaterials"

Non-ambient Pharmaceutical Studies 08:30 - 12:00 14th April 2005

Organisers: Anne Kavanagh & Roy Copley

Speakers include:
Dr Jonathan Burley (University Chemical Laboratory, Cambridge)
"Crystal Structure and Intermolecular Forces from Variable Temperature XRPD"
Jeremy K. Cockcroft (University College London)
"Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies"
Steve Cosgrove (AstraZeneca R & D, Charnwood)
"Probing (de)hydration behaviour by high resolution X-ray powder diffraction"
Francesca Fabbiani (University of Edinburgh)
"High pressure studies of pharmaceutical compounds"
Angus Forster (GlaxoSmithKline R & D, Stevenage)
"The use of X-ray diffraction in the pharmaceutical development of a dihydrate API"

Combined XRF/XRD Applications : 13:00 - 15:00 14th April 2005

See the Industrial Group Website for further details

Industrial Group and XRF 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 are offering a magnificent **prize of £50 and a bottle of Champagne** 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

For more information, contact:
Secretary/Treasurer

Future Meetings – Further Details

Two Day 2005 Autumn Programme

We are holding two back to back meetings in London this autumn. Day one is designed specifically to give a basic grounding in diffraction and its application in patents. Day two builds on this with a morning session related to patents and the afternoon on Crystallography in Industry. We expect that many people will attend both days but plan to offer separate registrations for each day to suit individual choice.

18th October 2005 Workshop on Patents in Crystallography

Organisers: Jeremy Karl Cockcroft & Anne Kavanagh.

This session will include tutorials on VERY BASIC PXRD, with lots of examples and the absolute minimum of theory. It is aimed at people who need to be able to understand about diffraction experiments but do not necessarily make diffraction measurements. The morning will provide many examples from a wide variety of research areas including industrial applications such as with polymorphs, amorphous versus crystalline components, impurity and mixed phases. The afternoon will provide a VERY BASIC introduction to the use of PXRD in patents with examples from both ceramic/mineral and pharmaceutical industries.

19th October 2005 Autumn Meeting "Patents & Crystallography in Industry", Birkbeck College, London.

Morning Session - Patents.
The morning theme will be "Patents" - a mix of presentations building on the previous days workshop organised by Anne Kavanagh and Richard Morris.

Afternoon Session - Crystallography in Industry.

The afternoon devoted to "Crystallography in Industry" - a diverse mix of presentations to cover a wide range of interests organised by Judith Shackleton and Steve Norval and will include a presentation on the recent Low Angle Round Robin.

Round Robin:
Registration for the Low Angle Round Robin will close on 30th April 2005. Results must be completed and returned by 31st May 2005
More details on our web pages.

If you measure peaks below 15° you should take part!

Newsletter Mailing

To keep cost down and to ensure that the newsletter gets to the appropriate people it is essential that we know your correct address. Also if there is a more appropriate contact in your organisation or if you no longer require a copy please let us know by contacting any of the committee officers.
The newsletter is also now posted on our WEB site (http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm) If you would like an e-mail notification of the WEB posting rather than a paper copy, then send an e-mail to djtaylor@lineone.net – with the title SUBSCRIBE WEB NEWS

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