BCA IG Newsletter

February 2006

EDITORIAL

This Newsletter is packed with details of our plans for 2006 and reports from our meetings last year. We have included a flyer on our XRF meeting in May with this issue that I hope you will pass on to your XRF colleagues Don't forget that we post the Newsletter on our web pages and maintain an archive going back to 1995.
The Spring meeting in Lancaster is a joint meeting with the British Association for Crystal Growth. It offers something for everyone using diffraction techniques even if it is only the opportunity to visit the vendors in the commercial exhibition or network with colleagues from around this country and beyond. There will be an Alun Bowen Lecture by Ulrich Griesser and an Industrial Group Award to Paul Fewster. A full day powder diffraction phase identification workshop offers an exceptional low cost training opportunity. A session on Neutron and Synchrotron opportunities for industrial users will introduce you to what these techniques can offer to extend your material characterisation possibilities. *Cont. on page 2.*

Inside This Issue

Forthcoming Events 2006

Spring Meeting 2006
4 - 6th April 2006 Lancaster University

10th May 2006 **XRF Meeting**, Keyworth.

8th June 2006 **Residual Stress** Workshop.

9th November 2006 **Autumn Meeting,**
Pilkington plc, Lathom, Lancs
Call for papers! more details on the web.
Log these dates in your diary NOW!

Provisional Diary Dates for 2007:
Spring Meeting 17-19th April 2007
venue to be confirmed.
Includes a full XRF programme and exhibition

XRF Newsletter 2 published electronically in January. View a copy on the web.

Industrial Group

BCA

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

Rigaku

Thanks **Rigaku** for sponsoring the cost of production and distribution of this edition of the Industrial Group Newsletter.

www.rigaku.com

Editorial continued.
There is a session on crystallisation and polymorphism of pharmaceuticals and a joint one with BACG on nanocrystallography. The session on Powder Diffraction in Industry will bring together a varied range of general interest talks. Please check out our web pages for the latest programme or to download a registration form. **The early registration deadline is 6th March.**

Our 23rd AGM is on Wednesday 5th April 2006 – see page 11 for details. Please note that the AGM agenda and draft minutes from the last AGM are now posted on the web in PDF format to give you the opportunity to view them well in advance of the meeting.

There will be more information on the web for our June Residual Stress Workshop and on the Autumn Meeting in our next newsletter, but now is the time for you to consider giving a talk at this autumn!

Also in this issue we launch a new Excel workbook based on some of the equations in the new European XRPD standards that I'm sure many of you will find useful.

We also have a preliminary update on the low angle round robin (LARR) based on a Silver Behanate film. You can now view the slides from the autumn meeting LARR presentation on the web.

Have you got something to say, a short technical article to offer, a website of the month to nominate or a puzzle for inclusion? If so the web editor is waiting to hear from you!

Do you have ideas for topics you would like us to cover in a future meeting? Just let any committee member know or even pick up the phone to discuss it with them – contact details are on the back page!

Sponsor this Newsletter!
Sponsorship of the distribution of around 400 copies of our next Newsletter is sought. Sponsorship offers good value and covers the full cost of distribution (approximately £200) – *contact the web editor for full details*.

2006 SPRING MEETING :
A FULL DAY XRPD workshop on Phase Identification. 4th April 2006
Tutors: *John Faber (Principal Scientist ICDD), David Rendle & Dave Taylor (consultants).* This is a modular workshop based on 4 distinct sessions. They build to give a complete understanding of phase identification and its progression into quantitative analysis, culminating in a flexible hands on computer session to gain practical experience with real examples. The modular structure will allow delegates, on the basis of their experience, to dip in an out of sessions through the day giving the package something to offer everyone with an interest in phase identification.

Module 1: 09:00 – 10:30 History & Structure of the Powder Diffraction File (PDF)
This module will cover important background information on the Powder Diffraction File with the emphasis on gaining an understanding of the various databases and how to interpret the data from an individual entry and select the best entry to use from multiple entries of the same compound.

Module 2: 11:30 – 12:00 Phase Identification
This module will cover collecting data for phase identification (PID). An understanding of the various manual search methods, alphabetical, Hanawalt, Fink and long 8 will underpin the knowledge required for automated search match techniques. It will cover selecting the database to use and subfile selection for particular applications.

Module 3: 13:00 – 15:00 Advanced Phase Identification and Quantitative Analysis.
Here we will cover data mining, total pattern analysis and the methods of quantifying the phases detected, covering reference intensity ratio, spiking and Rietveld analysis.

Module 4: 15:30 – 17:30 Hands on computer session. This module will allow you to put into practice the techniques covered in the workshop by using practical examples of both qualitative and quantitative problems for you to solve in a dedicated computer suite.

This one day workshop costs as little as £70 so why not take advantage and make sure someone in your organisation reaps the benefit!
Download a registration form from the web!

2006 Spring Meeting Lancaster University.
4-6 April 2006 Industrial Sessions.

SPRING MEETING - INDUSTRIAL PERSPECTIVE OVERVIEW			
	Tuesday 4th April	**Wednesday 5th April**	**Thursday 6th April**
AM	Phase Identification Workshop	Neutron & Synchrotron Opportunities. IG AGM	Nanocrystallography
PM	Phase Identification Workshop Exhibitors Forum	Alun Bowen Lecture Crystallisation & Polymorphism	Powder Diffraction in Industry. Including an IG Award
EVENING	Posters & Exhibition	Lonsdale Lecture Conference Dinner	

Wednesday 5th April

10:30 - 12:00 Neutron & Synchrotron Opportunities for Industrial Users
Session Chair: Jeremy Cockcroft

Examples of a wide spectrum of industrial uses of neutron and synchrotron facilities.

Alan Hewat, *ILL* - Title to be advised
Andrew Jupe, *Georgia Institute of Technology* - Title to be advised.

12:00 Industrial Group AGM

13:00 – 16:30 Crystallisation and Polymorphism of Pharmaceuticals.
Session Chairs: Roy Copley & Anne Kavanagh

Alun Bowen Lecture (Chair - Jeremy Cockcroft)
Ulrich Griesser, *University of Innsbruck*. - Relevance and Analysis of Polymorphism in Drug Development

Roger Davey, *University of Manchester* - Controlling nucleation of enantiomers from solutions - the chiral enrichment of mandellic acid.

Sally Price *UCL* - Progress and problems in computational prediction of crystallisation and polymorphism.

Terry Threlfall, *University of Southampton* Growing Crystals: Growing Polymorphs (and Some Thoughts on Crystal Growth)
Caroline Day, *GSK* - Polymorph Screening by Automated Techniques.

Thursday 6th April

11:00 -12:30 Nanocrystallography.

A joint session with British Association for Crystal Growth.
Sessions Chairs: Kevin Roberts (BACG) and Richard Morris (BCA)

Peter Laggner *(University of Gratz)* - How crystals are born: novel insight from small-angle X-ray scattering.

Kevin Roberts *(University of Leeds)* - Solution phase nucleation: cluster size & shape and its correlation with crystallisation kinetics and polymorph selection.

M Lal *(Liverpool University), M Plummer and W Smith (CCLRC)* - Metal nanocrystallites in supercritical fluids - the solvation process and its impact on the nanostructure.

13:30 - 16:00 Powder Diffraction in Industry
Session Chairs: David Beveridge & Judith Shackleton

This session will commence with an **Industrial Group award** to **Professor Paul Fewster** and continue with a diverse selection of industrial applications.
Other Speakers include:
David Beveridge, *Ilford PHOTO*. The Precipitation of Pigment Red 57:1 from Homogeneous Solution for X-Ray Powder Diffraction.

Chris Staddon, *Nottingham.* Title to be advised.

Meetings in 2006. (continued).
2005 Autumn Meeting reports

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 offers a magnificent **prize of £50 and a bottle of Champagne** for best poster.

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

Poster abstracts should be submitted on-line before 24th February 2006 at:
www.chem.gla.ac.uk/bca2006/

Get working on your industrial poster now!

Residual Stress Workshop

8th June 2006
VENUE to be confirmed.
Contact Judith Shackleton for more information.
Details will be posted on the web as they become available.

Autumn Meeting

9th November 2006.
At Pilkington plc, Lathom, Lancashire.

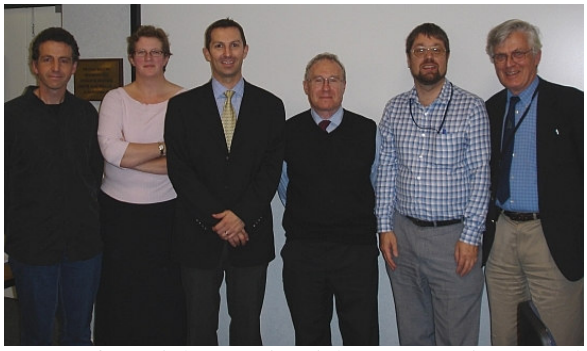
The theme for this meeting is:
Impact of Crystallography in an Industrial Environment.

Offers of talks should be discussed with the local organiser – Mark Farnworth.
(Contact details are on the back page)

Further details and some suggestions for presentations are on the meeting web page.

AUTUMN MEETING REPORTS

Workshop on Patents in Crystallography
18th October 2005
School of Crystallography,
Birkbeck College, London.



From Left to Right: Martin Vickers, Sam Price, Gareth Lewis, Mike Glazer, Jeremy K. Cockcroft and Bob Gould.

Samantha Towlson (Pilkington PLC)provided a refreshingly clear overview of patents covering the complete field from what a patent is, the benefits of owning one, what can be patented, how the process works, and concluding with some examples.

Jeremy Cockcroft (UCL/Birkbeck) lecture titled "Crystallography for Patents" covered information types in the context of patents and contrasted the information rich single crystal data, routinely collected at 150K, with the 1 dimensional data sets that may be obtained by XRPD. He highlighted the fact that the intensity information obtained using flat plate presentations is often inaccurate due to preferred orientation effects and that data collected using a transmission geometry was much more reliable. He advocated the sole use of peak position data in instances where the intensity data was unreliable and the use of indexing to confirm that the presented data was consistent with a single phase and pointed out that crystallographer often chose the unit cell on the basis of one whose angles are 90 degrees rather than necessarily the smallest volume.

Gareth Lewis (Astra Zeneca) provided an overview of the lead optimisation as applied within their company indicating that their preference was to develop a crystalline compound

based on a literature search that showed that of the 4700 drugs on the market only 7 are amorphous. He highlighted the importance of identifying the most stable crystalline modifications that a compound may exist in during the compounds early development. A small (and manual) polymorph screen is carried out internally and typically consists of 10-100 experiments. During late development it was then important to identify all the potential crystalline modifications:-

Solvent Mediated	Condensed phase
Solvent mediated wrt temp and time	Quench Cool from the melt
Recryst. wrt solvent properties and temperature. Typically using 6-20 solvents and 6-20 conditions.	Exposure to water vapour Pressure

A final polymorph screen of the most pure material from the final route of synthesis concludes the solid state form screen. Such screen appears to be carried out externally and typically consist of 100-1000 experiments. The methodology employed includes full structural characterisation using single crystal, XRPD and IR and then DSC TGA and hot stage microscopy. He explained the use of X-ray powder data to access non ambient data

X-ray is used both qualitatively and quantitatively through the use of characteristic peaks and pattern matching using le Bail/Pawley fit methods or Rietveld analysis which requires the single crystal data for the appropriate forms.

Martin Vickers(UCL/Birkbeck) provided an example of the type of data included in a patent application which demonstrated that the data may be of questionable quality; as in this case one of the diffraction patterns purporting to be a different solid sate form was consistent with the material simply exhibiting preferred orientation effects.

Jeremy Cockcroft (UCL/Birkbeck) provided an example where quantitative X-ray powder diffraction data had been used in a patent case in an attempt to demonstrate that one company was infringing another's patent on a livestock disinfectant which may contain sodium chloride at a levels as low as 0.025% as a result of the synthetic route based on the use of sodium dichloroisocyanurate. Using a method of standard additions it is possible to determine the concentration of the un-spiked material providing peak overlaps do not preclude this. Various presentation methods were considered and capillary was ruled out due to the relatively high background produced by the glass tube. Care in smoothing data is also indicated as his experience has shown that this may generate false peaks.

Mike Glazer (University of Oxford) lectured on crystallographic patents and seeding. He related his experience of being an expert witness and supplied his rules:

1. Do not lie.
2. Do not actively help the opposition.
3. Be aware of yourself and do not be tempted into discussion topics that you are not completely familiar with.
4. Talk slowly and consider carefully before making a statement.
5. Keep things simple.
6. Do not take with you to court any notes, papers or anything that you do not want the opposition to know about.
7. Do not make copious notes.
8. You are the expert.

He then cited a case in which the manufacture of a particular solid state form of Cephadroxyl monohydrate which is covered by a patent, that relates to a new method of synthesis, and material manufactured by the old process for which the

patent has lapsed. The work demonstrated that care has to be exercised in quoting characteristic peaks as if this is too loosely defined it is possible for the opposition to claim that they are making the original solid state form and not infringing your patent.
The highlight of the talk was a double act with Bob Gould re-enacting a transcript from an American court case, emphasizing the points made and demonstrating the aggressive nature of cross examination.

Philip Lake
GSK

"Patents & Crystallography in Industry" 19th Oct 2005

School of Crystallography, Birkbeck College, London.

Morning session - Patents.

From Left to Right: Chris Frampton, Richard Morris (chair) and Roger Savidge.

Chris Frampton (Pharmophix) talked on "Case Studies by an Expert Witness". Despite claiming not to be an expert at being an 'expert witness', Chris gave some excellent general advice on the duties and obligations of an expert witness. This included GLP (good laboratory practice), confidentiality, reporting and being prepared for unpleasant cross examination by the QC. Also how to give opinion within the boundaries of your remit, and being representative of peers in the XRPD industry, whilst avoiding the trap of being inventive yourself. He gave a couple of pharmaceutical examples, one of which was the classic tale of Paraxetine Hydrochloride, and the disappearing polymorph. It was noted that solvate forms, of which hydrates are a subset, are not polymorphs.

Roger Savidge (Consultant) then gave an insight into "Patents and Crystallography" from the users perspective, and cleared up some of the misconceptions. There are only national patents, although these can be applied for through regional (eg. European) or World (PCT) patent offices. The 20 year timescale was described, and the importance of keeping all the parts of your invention confidential until final application. In terms of exploitation, a granted patent does not give the inventor the exclusive right to exercise his invention, merely the right to prevent others. Thus in practice the patent holder, may *require* licenses from other inventors whose patents overlap in some way, and he may also *grant* a licence to others to use the invention commercially. You are not allowed in any way to threaten potential customers by suggesting that your competition may be infringing a patent. You are well advised to go through your solicitor.

Andrew Hodge
BP Chemicals.

Afternoon session: Crystallography in Industry

From Left to Right: Jeremy K. Cockcroft, Dave Taylor, Richard Stephenson, Judith Shackleton (chair) Steve Norval and Olivier Leynaud

Low angle Round Robin preliminary results, *David Taylor, consultant*

David opened by explaining that the purpose of

the Round Robin was to test the suitability of Silver Behanate to become a certified low angle intensity standard. The Round Robin would also provide direct intensity comparison between different equipment and set-ups and would provide participants with feedback on instrument performance. 21 users signed up for the Round Robin, to date 14 had returned data obtained from 17 instruments (1-Bede, 7-Bruker, 8-PANalytical and 1-Stoe). 22 data sets had been collected including 1 from Holland and 1 from Taiwan. All the data sets were obtained using copper tubes.

For comparing intensities, the data was normalised for 40mA current. 'Figure of Merits' were calculated for each data set. David said that some interesting information was coming through for example some users had quite high background counts at low angles. More data analysis will be carried out to explore affects due to slit size (variable VS fixed) and counting time. A full report will be published in due course and added to the Industrial Group's web pages.
See Page 11 for more details.

Standards, ***Steve Norval, ICI plc***

Steve updated the meeting on progress towards publishing the new European standards under the banner "Non-Destructive Testing - X-ray Diffraction from polycrystalline and amorphous materials".
Those so far published include:

- EN13925-1 - General Principles
- EN13925-2 - General Procedure
- EN13925-3 - Instruments

EN1330-11 - Terminology - is due to be published next year.
Future subjects include reference materials and phase identification and quantitative analysis.

Steve explained that XRPD in industry is used for understand materials, development of new materials, solving problems, identification, specification and attributing blame. Laboratories and departments need to communicate with customers and suppliers and need to conform to regulations and legislation. Thus, everyone needs to understand the technical language and XRPD users need to conform to international standards to obtain credibility. At a minimum there is a need for common concepts and terminology, well defined instruments, agreed reference materials, acceptable procedures and adequate reporting.

The committee is trying to produce structured standards with standards for overview/common issues, industrial techniques and specific applications. The three published standards to date cover general principles (basic concepts, Bragg equation etc), procedures and instruments. Terminology and Reference Materials standards are in progress and work on phase identification and quantitative analysis is starting. Standards could form the basis of laboratory accreditation and validation of patent data.

Neutron Diffraction - Introduction, ***Jeremy Cockcroft, Birkbeck College***
[The intended speaker Peter Laggner, Institute of Biophysics and X-ray Structure Research, Austrian Academy of Sciences was unwell and unable to attend. Jeremy stepped in to present a talk with the same title based on his presentation to the 2005 BCA Durham School].

Jeremy began by describing the properties of a neutron (mass 1, no charge, spin ½, strong interaction with nucleus, weaker interaction with unpaired electrons). Its kinetic energy is related to its velocity and temperature. Its coherent scattering cross-section gives rise to diffraction data - incoherent scattering contributes to the background signal.

Since neutrons interact with nuclei the point

2005 Spring Meeting Reports (continued)

In Situ: Processing in Industry.

scatterers are very small compared with the wavelength, unlike X-rays which interact with the electron cloud - Form Factor. The neutron pattern does exhibit decreasing intensity with 1/d. For neutron shielding, B_4C doped rubber, plastics or cadmium metal sheet is used. ^6Li is very good but is rarely used since in is normally extracted from the lithium containing ore for military use!

Detection relies on the absorption by the atomic nucleus with the simultaneous emission of a gamma-ray. ILL Grenoble is still Europe's highest flux neutron source. The reactor consists of 10g of ^{235}U surrounded by heavy water cooled to 35C. 'Hot' and 'Cold' sources produce long wavelength and short wavelength neutrons respectively. The neutrons are transmitted along nickel coated curved guides - Guide Halls. The beam from the reactor is a 'white' beam (continuous range of wavelengths). Selected wavelengths can be obtained by use of monochromators. The sample holders are high temperature quartz tubes. Overall, Jeremy gave a very interesting and comprehensive overview of the subject of Neutron Diffraction.

An in-situ study of a redox catalyst analysed by Rietveld refinement, *Olivier Leynaud, Birkbeck College*

In-situ diffraction arises from the need to understand what is happening inside the sample such as identification of intermediary compounds in a chemical reaction. Needs greater X-ray flux than produced by laboratory instruments so that quick reactions can be studied - Time resolved X-ray Diffraction. Olivier said that in order to meet these requirements, experiments are carried at Daresbury Laboratory's synchrotron source. The MPW 6.2PD station with RAPID 2 multi-wire detector (60degree range) is used. The small oven can be heated up to 950C and is water and air cooled. Vacuum experiments can also be carried out. The Fe-Mo-O catalyst system has been studied. An excess of MoO_3 in Fe-Mo-O has been found to be beneficial for the stability of the active phase and replenishing any sublimed Molybdenum. It allows the successful Rietveld refinement of the XRD patterns.

Structure Analysis of Novel-Templated ALPOs using CCP14 Software, *Richard Stephenson, UCL, Birkbeck College*

Novel-Templated ALPOs are a class of crystalline micro porous materials. Three synthetic mixtures produced the same layered structure. Introducing a cation e.g. Cobalt produced a different 3D structure i.e. poor reproducibility. Richard said that if single crystals are produced then it is possible to get comprehensive information from the refinement of their diffraction patterns. However, a particular issue is that the crystal is not representative of the bulk material. The refinement programs used can be viewed at the ccp14 web site (www.ccp14.ac.uk or www.ccp14.ac.uk/solution/xtalrefine/).

Crystals Software: Has an in-built wizard and there is guided structure refinement. A 'Supervisor' routine makes recommendations for further improvement. The refinement process can be followed with in-built graphics and electron density maps can be generated.

WINGX Suite for Windows: It is compatible with the Shelx range of programs. Resulting density maps can be viewed in Contour and Map view.

For structural refinement of powder diffraction data there is a large range of programs. However, they are not as sophisticated as those for single crystal data. They have the EXPQUI Interface for Rietveld programs such as Rietica, Ortex (image and movie animations) and Struplo for Windows (polyhedral structure drawings).

Mark Farnworth

Pilkington plc.

X-RAY FLUORESCENCE (XRF) PAGE

XRF Meeting 10th May 2006, at the British Geological Survey, (BGS) Keyworth, Nottingham.
Sponsored by: Ametek – Spectro, Analysco, BrukerAXS, HORIBAJobin Yvon Ltd, PANalytical and Rigaku.

We are pleased to announce that the BCA is collaborating with the **Royal Society of Chemistry, Atomic Spectroscopy Group** for this meeting. A flyer with more information on the meeting is included with this Newsletter; please pass on a copy to your XRF colleagues.

Offer a short talk! We are particularly keen to encourage XRF USERS to give short talks in the afternoon session at this meeting. Even if you have never given a talk in the past then this is your opportunity to make a short (10 minutes) presentation about what you do with XRF, share an experience or seek a solution to a problem. Contact any of our XRF team to discuss a contribution – see below for details.

Please make a special effort to attend this meeting and become part of a growing independent group of XRF users. Keep an eye on the meeting web page for the latest programme details.

Meeting Fees: £30 (£15 concessions) - open to non-members at no extra charge.
Registration will be on-line with a link from the web meeting page and will be available soon.

XRF Jobs Page
We have started an XRF jobs page on the web with links to UK jobs of interest to our members. Please let us know of any XRF jobs we should link on our page by following theinstructions on our Jobs Page.

Wanted: Mass attenuation Coefficients (mac)
Mac calculations are very useful in XRF - if you match the mac's of your samples and standards, calibration problems will be minimised. Calculating mac values from tabulated data is straightforward but tedious. You need to work out the mass fractions of individual elements in a mixture, and then multiply each of these by the appropriate mac value for the X-ray line of interest.

In the past, I've used a suite of rather elderly DOS programs. These work OK, but the system is limited by two factors:
1. Results are not stored (it originated with a system that printed it all out on a teletype).
2. The mac database has to be created by hand.
Needless to say, I've only input the data I'm most likely to use.

I'm creating a spreadsheet version that could in due course be made available on our web pages. This works, but the limiting factor is the mac database. Searching the web, I've found data for the K alpha and L alpha lines, but not for any other lines. To be comprehensive, I need data for absorbing elements down to at least uranium, for particular lines of particular radiating elements (a lot of the data available is by wavelength or energy but this is no use). This is a lot of data to type it in myself - typically 5500 - 6000 values per X-ray line.
So... does anyone know where I can get machine-readable tabulated data of mac values for K beta, L beta, M alpha or other lines?

David Beveridge
david.beveridge@ilfordphoto.com

WEB Newsletter – We run a web only XRF Newsletter, check the web for latest edition.

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Dates for 2007 17-19th April BCA Spring Meeting with a full XRF programme & Exhibition.

NEWS AND COMPETITIONS

Situations Vacant:
A jobs page for XRF and XRD positions is now operational on the IG Web pages. There is a link from the top of the IG Home page. Please submit any relevant job links you become aware of.

Sudoku:
Two solutions to the sudoku puzzle published in the last issue have been reported. Did you solve the puzzle?

Solution1 *(see web pages for solution 2)*

1	9	6	2	7	4	3	5	8
2	8	4	3	9	5	7	1	6
3	7	5	6	8	1	2	9	4
4	2	9	5	1	3	6	8	7
5	3	7	4	6	8	1	2	9
6	1	8	7	2	9	4	3	5
7	5	2	8	3	6	9	4	1
8	6	1	9	4	2	5	7	3
9	4	3	1	5	7	8	6	2

David Beveridge has supplied the following Sudoku puzzle for you to try.

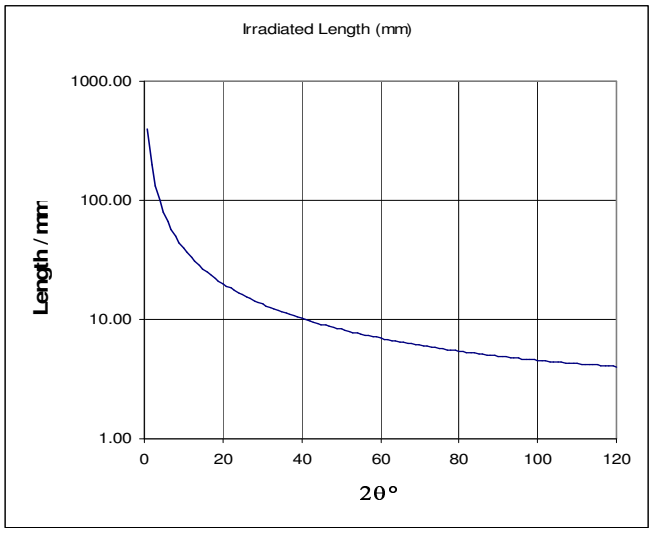
1		7		5		3		9
	5		3		9		4	
3		9		4		2		8
	7		5		2		9	
5		2				4		1
	9		4		1		8	
7		4		2		9		6
	2		9		6		1	
9		6		1		8		5

Excel Spreadsheet – available now.

Some of the Equations published in the European XRPD standards have been implemented in a Microsoft Excel workbook. The workbook consists of worksheets for each of the following:

- Braggs Law
- Irradiated Length
- Divergence Angle
- Specimen Height Displacement
- Infinite Thickness
- Mass Attenuation Coefficient

An example plot of irradiated length vs 2θ°



You can download the Excel file (which doesn't employ macros) from:
http://bca.cryst.bbk.ac.uk/bca/ig/Spreadsh/ENeqV1_0.xls

There are plans to convert further equations into the same spreadsheet format and we hope to have something available in time for our next Newsletter.

The file is made available through the BCA Industrial Group, as is and without warrany, by the joint authors:
Steve Norval, *ICI Measurement Science Group*
Dave Taylor, *consultant*.

NOTICES

Industrial Group AGM

The 23rd ANNUAL GENERAL MEETING of the Industrial Group will be held at Lancaster University at 12:00 on 5th April 2006

Nominations are sought to fill the following vacancies to serve for three years from April 2006.

-Vice Chair
-Secretary Treasurer
-THREE Committee Members

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.

The AGM agenda and draft 2005 minutes are on the web.

Web Site of the Month

Each month we feature a link to a web site of the month at the foot of the IG home page and the XRF home page. Please send suggestions for future featured sites to the IG Web editor. You can check sites previously listed on the archive page.

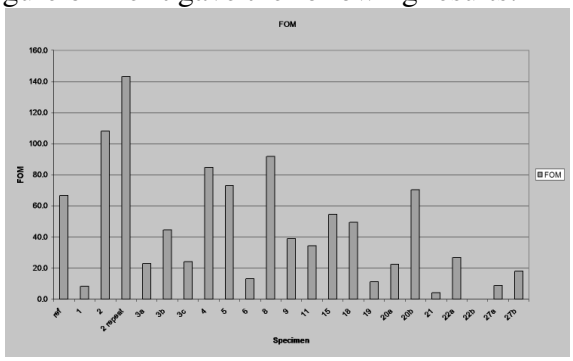
Industrial Group E-mail Mailing lists – Online registration.

We now maintain separate lists for XRF and XRD mailings so please register for BOTH if you want to be kept totally in the picture.

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 lists online - follow the link from the IG home page. There is an opportunity to be removed from the list with each mailing.

Low Angle Round Robin Update.

A preliminary report was presented at the Autumn Meeting. The presentation slides can be viewed on line at:
http://bca.cryst.bbk.ac.uk/bca/ig/present/LARRppt/Index.htm
A preliminary look at an intensity comparison figure of merit gave the following results:



The comparisons were made using crude inspection of the raw data files to extract peak positions, heights and widths manually. It is planned to rework the data with profile fitting techniques to give more accurate assessment of the data and allow evaluation of peak shape. The only correction to the data was to normalise all intensities to 40mA and more work is required to apply corrections for slit size, counting time, goniometer radius etc. Some problems were encountered in mounting the flexible film and with automatic specimen changers, resulting in specimen height problems. With care and the possibility of inverting the film to put the coating close to the specimen reference surface these problems can be largely overcome.
A preliminary evaluation of variability of the film coating across a sheet of the film is underway and differences have been observed. Work is ongoing to investigate variability of the film.
Some participants failed to submit data for evaluation, if they still wish to do so it will be added to the ongoing evaluation work.
A full report on this round robin will be produced in due course and be made available on the Industrial Group web pages.

Dave Taylor - January 2006

Industrial Group Committee
2004-2005

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