

# BCA IG Newsletter

August 2008

## Notes from the Chair

I'd like to start this Newsletter by welcoming new committee members, Matt Johnson and Brett Cooper, and to John Kaniuka who acts as a link between the Industrial Group and the Young Crystallographers.

Matt and Brett have really dived-in, and are organising this year's Autumn Industrial Group meeting, along with local organiser, Tal Austin. We are now in the throes of organising our part of the Spring 2009 meeting, and I'd like to encourage you all to consider offering to speak in one of our sessions.

On behalf of the IG committee I'd like to extend a big THANKYOU to our sponsors. Space does not permit them all to be listed here, but their names and logos can be found on our web site. The support we receive is really important to our activities and enables us to run meetings with very low delegate charges.

## Forthcoming Events

- 5th Nov 2008 **Autumn Meeting  
Pharmaceutical Special Interest Group**  
AstraZeneca, Loughborough
- 21st to 23rd April 2009  
**BCA Spring Meeting 2009**  
University of Loughborough

See the Industrial Group's web site for more details of these meetings.

**XRF Newsletter 7 published electronically in June 2008.** View a copy on the web.

## Inside This Issue

<b>1 - 2</b>	<b>Chair's welcome / Editorial</b>
<b>3 - 6</b>	<b>Spring Meeting 2008 - Reports</b>
<b>7 - 9</b>	<b>BGS May Meeting – XRF Reports</b>
<b>9 - 10</b>	<b>BGS May Meeting – XRD Reports</b>
<b>11</b>	<b>Forthcoming Meetings</b>
<b>12</b>	<b>Committee contact details</b>



Charity Registration Number: 284718

**World Wide Web addresses:**

**BCA** <http://www.crystallography.org.uk>

**IG** <http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm>

**Tip** Google BCA IG (with a space) to find us!

## THANK YOU



Thanks to **Rigaku** for sponsoring the cost of production and distribution of this edition of the Industrial Group Newsletter.  
[www.rigaku.com](http://www.rigaku.com)

The organisers of the May meetings on 'Minerals & much more!' took our tradition of low charges one step further by offering free places to students, thanks to generous sponsorship and the free use of the facilities of the British Geological Society. As always, the organisers, Martin Gill (XRD) and the XRF committee, came up with a great programs for the two days and 'much more' included a wine tasting, so that delegates could fully appreciate the impact of geology on viniculture. Another reason for all those happy smiley faces in the photos.

I'd also like to thank Rigaku for sponsoring this edition of the Industrial Group's Newsletter.

To conclude these remarks: many thanks to all those involved with this year's meetings, and I hope you have a great summer.

**Anne Kavanagh**  
Chair – Industrial Group

#### **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.

**Please sign up NOW!**

## **EDITORIAL**

Welcome to this edition of the BCA Industrial Group's Newsletter. It contains edited versions of Industrial Group reports for the BCA Spring 2008 meeting at the University of York and for the two-day Industrial Group meeting which was held at the British Geological Survey, Nottingham. Thank you to all those who attended these meetings and particularly to those who took time out from their busy lives to write-up the various reports. Please note that Spring Meeting Reports from other authors were published in the June edition of Crystallography News.

I would like to remind you that unedited versions of all the reports can be found on the Group's web site:

<http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm>

Our attention now turns to the Industrial Group's Autumn meeting. This will be a Pharmaceutical Special Interest Group meeting on the 5th November 2008 at AstraZeneca, Loughborough. The programme is coming together (see page 11) and there is now a Call for Papers. Contact the session Chairs for more information. The programme for next year's BCA Spring Meeting at Loughborough University is also being finalised. A flavour of the programme is also given on page 11. Please visit the Industrial Group's web-site for more information and updates as we get nearer to the event.

#### **Newsletter and Web Site Content**

We continually try to improve the content of both the Newsletter and web pages and would like to ask you to submit articles etc. Do you use web sites for your day to day work in XRD and XRF? If yes, then which sites do you visit, let us know and send us a paragraph about what you use the site for and why you like it. That's it for now. Enjoy your Newsletter.

**Mark Farnworth** – Pilkington Group Limited  
Editor

### **Applied Crystallography Showcase**

9th April 2008



**Speakers** - Left to Right: Back row - Chris Staddon (Chair), David Rendle, Mark Farnworth, Iain Oswald, Front row - Judith Shackleton, Suzanne Harte, Judit Debreczeni.

### **Industrial Group Young Crystallographers Prize Talk: High Pressure Structural Studies of Energetic Materials**

Iain Oswald, University of Edinburgh

Energetic materials release heat and / or gaseous products at a high rate on a certain stimulus e.g. heat, impact. Iain discussed high pressure studies of the beta polymorph (one of four) of HMX. Previous work had identified an alpha to gamma phase transition in which its space group, Pbc<sub>a</sub>, didn't change. Powder Neutron Diffraction shows that all the d-spacings contract, due to the pressure, and that Pbc<sub>a</sub> is not the correct space group. Attention turned to single crystal X-ray work. The space group was found to be Pca2<sub>1</sub> and there are two molecules with different conformations.

### **Direct Correlation between Ferrite Microstructure and Electrical Resistivity**

Judith Shackleton, University of Manchester

Ferrites are used for transformer cores and operate at ever increasing frequencies. Magnesium-zinc ferrites are toroid shaped. Judith showed results obtained from

Tomographic Energy Dispersive Imaging (TEDDI) which produces 3D scans of the lattice parameters calculated using the Le Bail full pattern method (TOPAS software). The lattice parameters were found to be larger on the outside of the samples. Resistivity measurements were also carried out and the variation in resistivity found to be about 10 ohm/cm over a length of approximately 800 microns. This is a similar length scale to that found by TEDDI.

### **Protein Structures in Drug Discovery – from Fragments to Macromolecules**

Judit Debreczeni, Astra Zeneca

Judit began by saying protein crystallography is one of the most powerful experimental techniques to aid the design and development of drug molecules in the pharmaceutical industry. It has been able to adapt to the ever-changing needs of the business, shifting focus on different drug targets and approaches. Robots are used for crystallisation and also for the crystallography e.g. crystal screening and data collection. High impact areas are studies for protein-ligand, protein-fragment and protein-protein interactions.

### **Applications of X-ray Diffraction and Mapping in the Glass Industry**

Mark Farnworth, Pilkington Group Limited

Glass making raw materials and the refractory materials that make up parts of the Float Glass Process are crystalline, so too are many ultra-thin coatings on glass. Mark described how the non-crystalline (or glassy) content of refractory material is determined. Thin coatings on glass can be highly textured. Pole-figure measurements to determine the strength of Ag(111) orientation in thin silver layers. In conclusion, Mark described how XRD maps are obtained from 10cm x 10cm coated glass plates. For a selected Bragg reflection, maps of peak area (a function of texture and layer thickness), peak position (a function of strain) and peak FWHM (a function of crystallite size) are measured.

### **Application of X-ray Diffraction and other Analytical Techniques to Pharmaceuticals**

Suzanne Harte, SAFC Pharmorphix

Suzanne explained why it is necessary to have a thorough understanding of the solid state properties of potential drug candidates. A wide range of complementary analytical techniques are used. By utilizing thermal, optical, spectroscopic and diffraction methods it is possible to gain a much greater comprehension of pharmaceuticals than can be achieved from one isolated technique. When a material first arrives spectroscopic Nuclear Magnetic Resonance (NMR) is used. High Performance Liquid Chromatography (HPLC) assesses purity and Aqueous Thermodynamic Solubility in water. A D8 GADDS instrument is used as a screening tool. Suzanne explained that it is a reliable method for identifying different forms of materials.

### **Application of X-ray Diffraction Within Forensic Science**

David Rendle (ICDD), Visiting Fellow (Cranfield Forensic Institute)

David began by saying that XRD has been used in forensic science laboratories around the world since before the middle of the last century. Its use sixty years ago was generally restricted to basic qualitative analysis. Modern day applications have the added advantages of the availability of high speed computer-controlled diffractometers and data processing software. *Intelligence gathering* – the recording and collation of detailed analytical results in a database – whilst time-consuming and tedious, is essential to the forensic scientist for estimating the significance of the results and for indicating trends over a period of time. David concluded by saying the analysis of street drug seizures by XRD yields not just the identity of the drug, but also the identities of the adulterants or excipients used to dilute the drug.

### **Small is Smart**

9<sup>th</sup> April 2008



**Speakers** - Left to Right: David Beveridge (chair), Steve Norval, Chris Gilmore, Chris Staddon

### **Powder Diffraction of Nanomaterials**

Steve Norval, Intertek MSG

Steve began by saying that, for the most part, techniques for phase identification, quantification, microstructure, in-situ monitoring etc are well established and were applied for decades before “nano” became fashionable. Heterogeneous catalysts are good examples of nanomaterials that have been around longer than X-ray Diffraction. Adsorbants and pigments were also being used before the nano-revolution. For a material to be described as ‘nano’ the crystal size in at least one direction is generally considered to be less than 100 nanometres. Stephen presented information about rutile titania, commonly used as a pigment in many materials. Crystallite size distributions determine its physical nature for example ‘white’ pigment is usually ¼ micron in size whereas for sun-block (scatters UV light) the pigment is approximately 25 nm. Nano-composite clays have enhanced mechanical properties and usually contain montmorillonite clays.



## 2008 Spring Meeting University of York - Reports

Full reports at <http://bca.cryst.bbk.ac.uk/bca/ig/rep08SM.htm>

### **X-ray In-Plane Scattering of GaN Nano-columns**

Christopher Staddon, University of Nottingham

Gallium nitride is a wide band gap semiconductor and is used in blue emission lasers, high density storage media and high power FET's. Chris said that a major problem with this material is the lack of suitable substrates, which in turn results in high defect densities in the material and hence less than ideal devices. To avoid this problem, isolated GaN nano-rods are grown by molecular beam epitaxy (MBE) on sapphire substrates using aluminium nitride buffer layers of appropriate thickness. Chris said that he has used in-plane scattering, to determine the mean value of the in-plane lateral dimensions, orientation and quality of the GaN nano-columns. The experimental data was collected from two independent in-plane reflections - (200) and (300). A bi-modal size distribution was discovered.

### **Solving Crystal Structures of Zeolites using Powder Diffraction and Electron Crystallography**

Chris Gilmore, University of Glasgow

Chris discussed zeolite structures and the challenges involved in solving them, particularly in early stages of synthesis and characterisation when samples are poorly characterised. The crystallite sizes are often so small that peak broadening makes the powder patterns hard to deconvolute. Chris has used density building functions and density histogram matching techniques to solve a number of structures ab-initio using both electron diffraction data in 2- and 3-dimensions and powder data. A low resolution structure is first generated using structure factors and more direct methods. They are analysed using density 'building'

functions. The optimal phase sets are subjected to entropy maximisation and then likelihood and density histograms are used to select the optimal phase sets.

### **Big is Beautiful**

9<sup>th</sup> April 2008



**Speakers** - Left to Right: George Bibby, Michael Drakopoulos, Judith Shackleton (Chair), Supriyo Ganguly.

### **Analysis of Weld Residual Stresses in Prototype Engineering Components and Structures using Pulsed Neutrons**

Supriyo Ganguly, Open University, Milton Keynes

Supriyo began by saying weld stresses can result in fatigue so there is a requirement to investigate damage tolerance. This has been carried out through the WELDES project. Welding is probably more cost effective than traditional riveting. The factors which control fatigue initiation and crack growth are well known but it is important to understand the actual crack growth mechanism. Two aluminium alloys have been investigated: 2024-T351 and 7150-T651. Wing structures are machined and welded. The size and measured density define the appropriate residual stress measurement that is used. Time-of-Flight Diffraction with a 14-40 millisec range and Pulsed Neutron Strain Scanning are techniques that have been used.

## 2008 Spring Meeting University of York - Reports

Full reports at <http://bca.cryst.bbk.ac.uk/bca/ig/rep08SM.htm>

### **Residual Stress Measurements of gas turbines components by X-Ray Diffraction**

George Bibby, Rolls Royce

Residual Stress measurements are made to effect the quality control in material supply. George discussed the method of manufacture of cast / wrought discs and the architecture of gas turbines. They have analysed low pressure compressor blades, high pressure turbine discs and engine mounts. Components can be immersed in hydrofluoric acid to remove surface material prior to analysis. Sources of error include 'psi splitting' due to the presence of 'out of phase' shear forces and shadowing due to material on the sample that impinges the diffraction cones. George concluded by saying that providing the methodology is right then X-ray diffraction is a very satisfactory method for measuring residual stress.

### **JEEP: The Joint Engineering, Environmental and Processing Beamline at Diamond Light Source**

Michael Drakopoulos, Diamond Light Source Limited

Michael informed everyone that DLS is constructing a beamline dedicated to Engineering Science. It will be the first engineering beamline in the UK. The beamline will focus on diffraction and imaging-based methods for the study of structural properties of engineering materials in static and dynamic conditions. Imaging and tomography provide structural information a microscopic scale. For deep penetration into materials, JEEP will provide synchrotron radiation at X-ray energies between 50keV and 115keV (0.28 to 0.08 angstroms). The attenuation length for iron is a few millimetres at 3x the attenuation length the signals are still strong so measurement through 1cm of steel will be possible.

### **IG Plenary Lecture**

9<sup>th</sup> April 2008

#### **X-ray Diffraction on Mars**

Rob Delhez – Delft University of Technology



**Speakers** - Left to Right: Anne Kavanagh (chair), Rob Delhez.

Rob began by saying that space research is driven by curiosity or scientific interest in many fields. If there is life in space we need to find organic molecules. Humankind has found 150 molecular species in the space environment, 230 including isotopes. Of these, 50 species have been found in comets. For meteorites approximately 3% of the mass is organic of which 20% is soluble and 80% is kerogene. Unlike the Earth, Mars has no tectonic plates and no magnetic field. A Mars Science Lab will contain X-ray Diffraction and X-ray Fluorescence instruments. The mission has several goals including the search for life, climate and geology investigation and human exploration. Projects are also planned to investigate organic materials. Some minerals/structures are formed by algae e.g. banded iron formation (BIF) and stromatolites (calcium carbonates). Other can host organic molecules e.g. iron hydroxides and clay minerals. Rob concluded by explaining the requirements of a Mars XRD instrument.  
*Mark Farnworth, Pilkington Group Limited*

**XRF: Minerals and much more!** (see web-site for all the reports)  
British Geological Survey, Keyworth, Nottingham, 14th May 2008



### **Morning Sessions**

The first talk of the morning was by **Nick Marsh (Leicester University)**, on the preparation and presentation of mineral samples for XRF analysis. The usual requirement is a fine powder and there are several stages to get this. Drying should be undertaken with care: volatile elements such as mercury can be lost, as can essential water from hydrated minerals. Crushing and milling is very dependent on hardness, brittleness, cleavage and density, all but the last of which can be anisotropic. The final stage is to convert the powder into a form suitable for analysis. This may be a loose powder, a pressed pellet, a fused bead, even a dust on a filter.

**John Mansell (Omya UK Ltd)**, who spoke about the analysis of limestones by EDXRF. This study included elements from major to trace levels, and included samples from a large number of quarries, so that the provenance of unknown samples could be established. The XRF method was very much quicker than previous methods (ICP or DCP-based) which required preliminary dissolution of the sample.

**Margaret West (West Analytical Solutions Ltd)** described a new BSI standard for glass-making sands. She described the parameters of the specification for a glass-making sand, and how the new version of BS2975 had been put together by the Society for Glass Technology. This is in two parts: sampling and testing; and chemical analysis. A wide range of physical properties is specified, which need to be tested. There is a detailed description of a sampling protocol, because sampling (surprise, surprise!) is one of the trickiest problems in the analysis. Grinding media were also discussed.

**John Boyle (University of Liverpool)**, who described the analysis of lake sediment cores by EDXRF. These samples can be very variable, and a general approach is needed. Many elements must be determined, often in a small sample (less than 1 g - the cores may have to be divided among many researchers). Particle size is rarely a problem because it is normally very small anyway. Matrix effects are definitely a problem, but one for which corrections can usually be made. Background measurements can be awkward, as the peaks are close together.

*David Beveridge, Harman Technology limited*



**XRF: Minerals and much more!** (see web-site for full reports)  
British Geological Survey, Keyworth, Nottingham, 14th May 2008

### **Afternoon Sessions**

**Neil Eatherington, (British Geological Survey, Nottingham)** Neil acknowledged that for the majority of applications XRF requires sample preparation to get the best from the technique, but what happens when preparation is not an option? Drying of samples was discussed with attention drawn to the problems of using a microwave oven and the loss of volatile analytes from environmental and soil samples. Conventional drying was ruled out because of the time taken to achieve a dry sample measured in days rather than minutes. Several case studies were presented featuring marine sediment cores, panned stream concentrates and in-situ analysis.

**Prof Graham Martin, (Victoria and Albert Museum, London)**

This was a different presentation where Graham avoided posting the usual spectra, graphs and data but instead concentrated on the application of ED-XRF within the heritage sector. Graham began with an overview of the Victoria and Albert Museum and its associated institutes and explained that a large challenge was communicating the applications to his colleagues with arts based backgrounds. The sheer scale and diversity of the exhibits and potential sampling sites were discussed together with the fact that invasive and chemical techniques were offered as a last resort but usually not at all.

*Simon Carter, BGS*

**Owen Butler, (HSL, Buxton)**

Owen began by summarising the work of the HSL at the Buxton site which has favourable scientific and engineering facilities. As an agency of the Health and Safety Executive, part of the governments Department of Work and Pensions the analytical services unit undertakes wide ranging tests and is involved with regulatory and investigative measurements.

In particular was noted the problem caused by ergonomic work practices of sampling to mimic inhalation. A new model for sampling particles, the Minisampler employing a 13 mm filter located adjacent to the mouth was demonstrated and validated using a model and automated welding rig. Elke introduced her work with VMM, the Belgium equivalent of the EA, reporting on air and water quality and the general state of the environment. Air quality was measured in a network of automatic and semiautomatic stations for a variety of parameters including PM10 and PM2.5 particulate fractions. Elke went on to describe the equipment used for heavy metal determinations commenting on the inflexibility of using two X-ray tubes for the WD-XRF technique.

**Richard Meeres, (Bureau of Analysed Samples Ltd)**

This presentation discussed the history of the company, from its inception in 1912 as Ridsdale & Co to the Bureau of Analysed Samples (BAS) in 1935. In 1950, the Honorary Advisory Committee (HAC) was created to provide an unbiased wealth of experience, make recommendations, evaluate results and approve Certified Reference Materials (CRMs). The HAC has met twice a year since its creation, and BAS also organises Triennial Meetings of UK Co-operating Analysts to gather comments and ideas for the future. The types of CRMs produced consist of iron & steels, non-ferrous metals & alloys, iron & non-ferrous ores, ferro-alloys, slags & refractories and ceramic materials & minerals.

**Alison Burke, (Huntsman Pigments)**

Huntsman Pigments has seven factories around the world which together produce approximately half a million tonnes of titanium dioxide each year. Around 60% is used in coatings (paint, etc) with the remainder being used in products



**XRF: Minerals and much more!** (see web-site for all the reports)  
British Geological Survey, Keyworth, Nottingham, 14th May 2008

such as plastics, inks, toothpaste and cosmetics. Several techniques are used for elemental determination; however XRF provides a simple, rapid and easy to use method. The Harmonisation Project of Analysis was initiated in 1998 in order to ensure inter-site reproducibility precision targets for each XRF element. Initially blind testing was carried out every six months to establish levels of agreement using z-score statistics.

**Andy Scothern, (Saint-Gobain Gypsum)**

Gypsum markets consist largely of construction (37%), renovation (29%), household (19%) and industry (15%). Saint-Gobain Gypsum (SGG) currently employs in excess of 200,000 people. Research and Development centres are based mainly in France. Gypsum consists of several phases -

gypsum ( $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ ), hemi-hydrate ( $\text{CaSO}_4 \cdot 1/2 \text{H}_2\text{O}$ ), and both soluble and insoluble forms of anhydrite ( $\text{CaSO}_4$ ). By applying temperature to this material, it phases through gypsum to hemi-hydrate to soluble anhydrite finally to insoluble anhydrite and back again by the addition of water. Samples are dried overnight at  $40^\circ\text{C}$  in order to remove any free water and to convert any soluble anhydrite to hemi-hydrate.

*Leian Grimsley BGS*

**Call for Papers – XRF Programme  
2009 BCA Spring Meeting**

If you already have a talk in mind then please send a title and brief description ASAP for consideration to the session chair – see web-site for more information

**XRD and Minerals** (see web-site for all the reports)  
British Geological Survey, Keyworth, Nottingham, 15th May 2008



**Morning Presentations**  
**Caroline Kirk, Loughborough University**  
**and the Department of Mineralogy,**  
**Natural History Museum,** gave a talk on

the Structural Studies and High Temperature Properties of Bismuth Vanadate Sillenites. Caroline explained that phase formation in the bismuth-rich end of the  $\text{Bi}_2\text{O}_3\text{-V}_2\text{O}_5$

**XRD and Minerals** (see web-site for all the reports)  
British Geological Survey, Keyworth, Nottingham, 15th May 2008

system had been investigated and an extensive solid solution of sillenite related phases found four temperature dependant polymorphs. It was found using DTA and impedance spectroscopy that conductivity also varied with changes in temperature. X-ray diffraction experiments with increasing temperatures show that at 750°C the system transforms from BCC to FCC and on cooling from FCC to BCC at 650°C. On cooling there are 2 BCC phases, which are metastable - why? Perhaps there is a problem with the structure model.

**Stephen Cairns, WestCHEM, University of Glasgow** discussed the importance of the understanding of the structure of ettringite and thaumasite in the application of civil engineering, specifically in the complex reactions of concrete.

The formation of ettringite in setting concrete, leads eventually to the formation of cracks - a famous example of this being the collapse of the Kepong Bridge in Malaysia. The ettringite group of minerals have the general formula  $\text{Ca}_6\text{X}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$ , where X = Al, Cr, Fe and Si and the sulphate group can be substituted by carbonate or borate groups. Although compositionally similar they are structurally different.

### Afternoon Sessions

**Stephen Hillier, Macaulay Institute**, gave a presentation on the second survey of the National Soils Inventory of Scotland (NSIS). This included an overview of the importance of soil to the ecosystem and how it is affected by its mineralogy. Scottish soils differ from the rest of the UK in that they have a higher organic content, lower pH and are lower in nutrients.

**Andrew Hardy**, followed with a talk about cosmeceuticals. He explained that these are compounds that combine both pharmaceutical properties with a cosmetic role. Their first recorded use is believed to have been by the ancient Egyptians. A bivalve shell dated from 1300BC has been found containing traces of a green compound believed to be copper based.

**Alison Pawley** discussed synchrotron studies of the structure of hydrous phyllosilicates (HPs) at high pressure and temperature. HPs are important in the Earth's mantle. They occur at subduction zones and take part in recycling water back in to the mantle. This water then affects the flow rheology of the mantle. HPs are soft and highly anisotropic. An example is talc, a magnesium silicate hydrate, which exhibits weak stable sliding behaviour. By increasing the pressure talc transforms in to a 10 angstrom phase that is likely to be involved in the transport of water in to the mantle to depths of up to 200km.

There is an international study taking place on crystalline silica. The reasons for this and the use of XRD in this study was presented by **Peter Stacey** in a presentation entitled accuracy in analysis - how much crystalline quartz do you think you have? Crystalline silica causes silicosis therefore there is legislation related to its measurement. Samples of dust are taken from the air and collected on mini filters. These are then placed directly in an Xpert Pro MRD.

The final talk of the day was given by **Melanie Sapsford** on analysis of non-marine evaporitic deposits of the Wadi Natrun in Egypt. Examination of the geological and archaeological samples helps to determine the role that sodium salts have played in ancient Egypt and how these relate to the changing nature of the Wadi lakes.

*Alison Burke, Huntsman Pigment*

## Forthcoming Meetings

### Autumn Meeting Pharmaceutical Special Interest Group

**5<sup>th</sup> November 2008**

AstraZeneca, Charnwood Site, Loughborough

Chaired by **Anne Kavanagh, Brett Cooper**  
and **Matthew Johnson**.

Speakers at this meeting will be:

**Robert Docherty, Pfizer:** The Future  
Application of Computational Methods in Solid  
Form Selection.

**Graeme Day, University of Cambridge:**  
Discovering and Understanding New Crystal  
Forms: Guiding Experiments by Crystal  
Structure Prediction and Modelling

**Frank Leusen, University of Bradford:** A Major  
Advance in Crystal Structure Prediction

**Xue Wang, University of Leeds:** Crystal  
Morphology: Measurement, Modelling and  
Closed-loop Control

**Amy Robertson, AstraZeneca:** Process  
Analytical Technology Applications in  
Crystallisation Development

**Claire Thompson, GlaxoSmithKline:**  
Pharmaceuticals in a State of Disorder - But  
How Much?

**Matt Tucker, ISIS:** Looking Beyond the Bragg  
Peaks with Total Scattering

For travel directions see:

<http://bca.cryst.bbk.ac.uk/bca/ig/Trav08AM.htm>

Organisers:

Dr. Matthew Johnson:

[matthew.6.johnson@gsk.com](mailto:matthew.6.johnson@gsk.com)

Dr. V. Brett Cooper:

[brettcooperhome@btinternet.com](mailto:brettcooperhome@btinternet.com)

### BCA Spring Meeting 2009

University of Loughborough, 21-23<sup>rd</sup> April

### Industrial Group Contributions

Plenary: ***Environmental Analysis with XRF  
and XRD*** Nick Marsh (Leicester)

Wed 22<sup>nd</sup> April

Chair: Anne Kavanagh

**Joint XRF and XRD session on  
Environmental Analysis**

Wed 22<sup>th</sup> April

Chair: Dave Taylor/Richard Morris

**Joint IG/BACG Session 1: Monitoring  
crystals, crystallization and transformations**

Wed 22<sup>th</sup> April

Chair: Nick Blagden (BACG)

**Joint IG/BACG Session 2: Monitoring  
crystals, crystallization and transformations  
- including the IG YC prize talk**

Wed 22<sup>th</sup> April

Chair: Alison Burke

**Understanding API Phase Transitions**

Thu 23<sup>rd</sup> April

Chair: Brett Cooper

**Crystallography in the Pharmaceutical  
pipeline**

**Thur 23<sup>rd</sup> April**

Chair: Matthew Johnson

**Industrial Group AGM**

11:45 Wed 23<sup>rd</sup> April

The 26<sup>th</sup> ANNUAL GENERAL MEETING

The meeting also includes a full three days of  
XRF sessions. More information and details of  
other sessions will be available soon on the  
BCA web-site meeting page.

## Industrial Group Committee 2008-2009

### Chair:

**Dr A M Kavanagh** – Anne

Tel: 01625 517454

Email: IGChair.BCA@googlemail.com

### Vice Chair:

**Mr R C E Morris** – Richard

Tel: 0121 544 7912

Email: max.13@btconnect.com

### Treasurer:

**Dr D Beveridge** - David

Tel: 01565 650000 Fax: 01565 872734

Email:

david.beveridge@harmantechnology.com

### ***Please address all official Industrial Group correspondence to:***

BCA Industrial Group Treasurer, Dr David Beveridge, Brentwood, Woodford Road, Poynton, STOCKPORT, Cheshire. SK12 1EG

### Secretary:

**Mr M Gill** – Martin

Tel: 020 7942 5920

Email: m.gill@nhm.ac.uk

### Committee Members:

**Ms J Shackleton** – Judith

Tel: 0161 200 3581

Email: judith.shackleton@man.ac.uk

**Mr C R Staddon** - Chris

Tel: 0115 951 5181

Email: chris.staddon@nottingham.ac.uk

### Newsletter Editor

**Mr M A Farnworth**, - Mark

Tel: 01695 54639

Email: Mark.Farnworth@pilkington.com

**Dr A E Burke** – Alison

Tel: 01642 376540

Email: alison\_e\_burke@huntsman.com

**Dr V B Cooper** - Brett

Email: brettcooperhome@btinternet.com

**Dr M Johnson** - Matthew

Email: matthew.6.johnson@gsk.com

### Co-opted:

Dr. S V Norval - Steve

Tel: 01642 435736

Email: steve.norval@intertek.com

### ICDD Representative (*Ex officio*) & IG Webmaster

**Mr. D J Taylor** – Dave

Tel: 01744 893108

Email: djtaylor@lineone.net

### Young Crystallographer Representative

**Mr. J Kaniuka** – John

Tel: 01695 54303

Email: john.kaniuka@pilkington.com

## XRF Organising Committee

**Mr Dave Taylor**

Tel: 01744 893108

Email: djtaylor@lineone.net

**Dr David Beveridge**

Tel: 01565 650000 Email:

david.beveridge@harmantechnology.com

**Mrs Margaret West**

Tel: 0114 2490517

Email: margaretwest@blueyonder.co.uk

**Mr Mark Ingham**

Tel: 0115 936 3341

Email: mni@bgs.ac.uk

**Dr Ros Schwarz**

Tel: 01777 702345

Email: rschw2345@aol.com