

## BCA 2005 SPRING MEETING: SCIENTIFIC PROGRAMME

**Tuesday 12 April**

**CC.00.11: 10.45 – 12.30**

**10.45 Welcome and short report from the President: Chick Wilson**

**PLENARY SESSION: In situ and Non-ambient Crystallography**

Chair: John Finney (UCL)

11.00 Phil Coppens (SUNY Buffalo, USA)

*X,Y,Z and time: introducing the time dimension in crystallographic research*

11.45 John Rafferty (Sheffield)

*Structural studies of DNA Holliday junction resolvases*

**12.30 Lunch, Exhibition and Posters**

**CC.00.11: 13.30 – 15.00**

**PLENARY SESSION: In situ and Non-ambient Crystallography**

Chair: Paul Raithby (Bath)

13.30 Herbert Pöllmann (Halle, Germany)

*XRD, XRF and in-situ investigations on anhydrous and hydrous cementitious materials - some examples*

14.15 Malcolm McMahon (Edinburgh)

*Pressure induced complexity in the elements*

**15.00 Tea and Exhibition**

**Exhibitors include:**

Hiltonbrooks  
Analysco  
Spectro  
Bruker  
Socachim- Xrf Scientific  
Genomic Solutions  
PANalytical  
ICDD  
Fluidigm  
Molecular Dimensions  
Perkinelmer Las  
Oxford Instruments  
Spex Certiprep  
Beevers Miniature Models  
Oxford Diffraction  
Rigaku  
Horiba Jobin Yvon  
Marresearch  
Oxford Cryosystems  
Malvern Instruments  
Taylor & Francis  
Oxford University Press  
CyBio

**CC.00.11: 15.30 – 16.00 Tuesday 12<sup>th</sup> April**  
**PARALLEL SESSION: CCDC/CCG Prize Award and Lecture**  
Chair: Sandy Blake (Nottingham)

15.30 The CCDC/CCG Prize for Younger Scientists:  
Anders Markvardsen (ISIS)

**CC.00.11: 16.00 – 18.00**

**PARALLEL SESSION: Crystallography Exhibitors Forum**  
Chair: Chick Wilson (Glasgow)

16.00 Exhibitor presentations:  
*Short commercial presentations by XRD exhibitors will give delegates a chance of updating their product knowledge and prioritise their visits in the exhibition.*

Talks include, but may not be limited to, presentations by the following Exhibitors:

- Fluidigm
- ICDD
- Malvern Instruments
- Marresearch
- Molecular Dimensions
- Oxford Cryosystems
- Oxford Diffraction
- PANalytical
- Rigaku

18.00 Close

**CC.00.13: 15.30 – 18.00**

**PARALLEL SESSION: XRF and XRF Exhibitors Forum**  
Co-Chairs: David Beveridge (Ilford Imaging UK);  
Dave Taylor (BCA)

15:30 Dave Taylor (BCA)  
*Introducing XRF – what is it and what can it do?*

16:00 Phil Russell (PANalytical)  
*What XRF for which job?*

16:30 Exhibitor presentations  
*Short commercial presentations by XRF exhibitors will give delegates a chance of updating their product knowledge and prioritise their visits in the exhibition.*

Talks include, but may not be limited to, presentations by the following Exhibitors:

- Analysco
- Bruker
- Horiba Jobin Yvon
- Oxford Instruments
- PANalytical
- Rigaku
- Socachim-Xrf Scientific
- Spectro
- Spex Certiprep

18.00 Close

**Exhibition Hall: 18.30 – 22.00 Tuesday 12<sup>th</sup> April**

**Poster Session and Exhibition, with Buffet Dinner and Wine Reception**

**Wednesday 13 April**

<p><b>CC.00.11: 08.30 – 10.00</b></p> <p><b>In situ Diffraction</b> Chair: John Evans (Durham)</p> <p>08.30 Matt Rosseinsky (Liverpool) <i>In-situ diffraction in inorganic materials discovery and processing</i></p> <p>09.00 Poul Norby (Oslo) <i>In-situ synchrotron studies probing the synthesis/application of inorganic materials</i></p> <p>09.30 Roger Davey (UMIST) <i>Using x-rays for the in situ study of crystallisation processes</i></p>	<p><b>CC.00.14: 08.30 – 10.00</b></p> <p><b>Photocrystallography</b> Chair: Paul Raithby (Bath)</p> <p>08.30 Jacqui Cole (Cambridge) <i>Single-crystal X-ray diffraction studies of photo-induced molecular species</i></p> <p>09.15 Judith Howard (Durham) <i>Spin cross-over complexes: structures and photomagnetism of high spin, low spin and metastable states and the LIESST effect</i></p>	<p><b>CC.00.12: 08.30 – 10.00</b></p> <p><b>At and in the Membrane</b> Chair: Steve Prince (Manchester)</p> <p>08.30 Steve Baldwin (Leeds) <i>Membrane protein expression in the genomic era</i></p> <p>09.00 Piet Gros (Utrecht, Netherlands) <i>Two outer-membrane proteins: translocation through a narrow beta barrel pore and a tilted beta barrel</i></p> <p>09.30 Bob Stroud (UCSF, USA) <i>A two billion year old tale of membrane transport: ‘gas’ channels and water channels</i></p>	<p><b>CC.00.13: 08.30 – 10.00</b></p> <p><b>XRF: Liquid samples.</b> Chair: David Beveridge (Ilford Imaging UK)</p> <p>08.30 Siân Shore (Shell Global Solutions) <i>Overcoming cobalt interference in sulphur analysis</i></p> <p>08.50 Al Martin (RigakuMSC) <i>Ultra carry filter, allowing ppb detection levels by WDXRF</i></p> <p>09.10 Gaetan Deshais (BrukerAXS) <i>Film 2005. A review of thin films used in XRF analysis of liquid samples</i></p> <p>09.30 Steve Davis (PANalytical) <i>Using Activated Alumina for Heavy Metal Contaminants Analysis</i></p>
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**10.00 Coffee, Exhibition and Posters**

<p><b>CC.00.11: 10.30 – 12.00</b></p> <p><b>In situ Processing in Industry</b> Chair: Steve Norval (ICI)</p> <p>10.30 Gordon Tiddy (Manchester) <i>Surfactant formulation</i></p> <p>11.00 Geoff Moggridge (Cambridge) <i>Processing block co-polymers for nano-pores</i></p> <p>11.30 Simon Jacques (UCL) <i>In situ crystallisation studies of pharmaceutical materials</i></p> <p>-----</p> <p><b>12.00 – 12.30 AGM: Chemical Crystallography Group</b> Chair: Sandy Blake (Nottingham)</p>	<p><b>CC.00.14: 10.30 – 12.00</b></p> <p><b>Photocrystallography</b> Co-Chairs: Paul Raithby (Bath); John Helliwell (Manchester)</p> <p>10.30 Eric Collet (Rennes, France) <i>The key role of X-ray diffraction for the investigation of photo-induced phase transitions</i></p> <p>11.05 Beatrice Vallone (Rome, Italy) <i>Protein structural dynamics observed by time resolved crystallography</i></p> <p>11.40 John Helliwell (Manchester) <i>The 15K neutron structure of saccharide-free concanavalin A</i></p> <p>12.00 Lunch, Exhibition and Posters</p>	<p><b>CC.00.12: 10.30 – 12.00</b></p> <p><b>Modern Techniques for Crystal Structure Refinement</b> Chair: Charlie Bond (Dundee)</p> <p>10.30 Richard Cooper (Oxford) <i>Advanced techniques in structure refinement</i></p> <p>11.00 Thomas Schneider (Milan) <i>Refinement of proteins as large small molecules using SHELXL</i></p> <p>11.30 Garib Murshudov (York): <i>REFMAC: recent developments towards automatic refinement</i></p> <p>12.00 Lunch, Exhibition and Posters</p>	<p><b>CC.00.13: 10.30 – 12.00</b></p> <p><b>XRF Workshop: Awkward Samples</b> Chair: David Beveridge (Ilford Imaging UK)</p> <p>10.30 Awkward samples workshop <i>An informal session for sharing problems and solutions</i></p> <p>12.00 Lunch, Exhibition and Posters</p>
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Wednesday 13 April 12.00 Lunch, Exhibition and Posters			
<p><b>CC.00.11: 13.00 – 13.30</b></p> <p><b>AGM: Physical Crystallography Group</b> Chair: Pam Thomas (Warwick)</p> <p><b>13.30 – 15.00</b> <b>In situ Diffraction</b> Chair: Andrew Harrison (Edinburgh)</p> <p>13.30 Pam Thomas (Warwick) <i>Synchrotron X-ray studies of ferroelectrics under applied electric fields</i></p> <p>14.00 Mark Smith (Warwick) <i>The use of in situ diffraction to probe the processing of amorphous silicate-based materials from gelation to reaction with biofluids</i></p> <p>14.30 Rudolf Winter (Aberystwyth) <i>In-situ small angle X-ray scattering study of interface morphology in sintered nano-ceramics</i></p> <p>14.45 Amber Thompson (Durham) <i>In-situ diffraction studies of spin crossover coordination polymers</i></p> <p>15.00 Tea, Exhibition and Posters</p>	<p><b>CC.00.14: 13.00 – 14.30</b></p> <p><b>Crystallography in Industry</b> Chair: Judith Shackleton (Manchester)</p> <p>13.00 Michael Preuss (Manchester) <i>Residual stresses in friction welded aeroengine components</i></p> <p>13.30 Tony Fry (National Physical Laboratory) <i>Residual stress measurements at NPL. Increasing confidence and developing best practice</i></p> <p>14.00 Martijn Fransen (PANalytical) <i>Title TBA</i></p> <p>14.30 Tea, Exhibition and Posters</p>	<p><b>CC.00.12: 13.00 – 14.30</b></p> <p><b>Modern Techniques for Crystal Structure Refinement</b> Chair: Simon Parsons (Edinburgh)</p> <p>13.00 Charlie Bond (Dundee): <i>What's that blob? Identifying metal ions in protein crystal structures</i></p> <p>13.30 Bill David (ISIS) <i>Beyond least squares</i></p> <p>14.00 Alan Coelho (ISIS) <i>TOPAS-Academic, programming ideas</i></p> <p>14.30 Tea, Exhibition and Posters</p> <p>-----</p> <p><b>CC.00.12: 14.30 – 14.45</b></p> <p><b>AGM: Biological Structures Group</b> Chair: Richard Pauptit (AstraZeneca)</p> <p>14.45 Tea, Exhibition and Posters</p>	<p><b>CC.00.13: 13.00 – 14.30</b></p> <p><b>WDXRF Applications.</b> Chair: Mark Ingham (British Geological Survey)</p> <p>13.00 Margaret West (West X-ray Solutions Ltd) <i>Keeping it clean</i></p> <p>13.30 David Beveridge (Ilford Imaging UK Ltd) <i>Determination of sulphur and chlorine in organic compounds by XRF</i></p> <p>14.00 Michel Davidts (Socachim-XRF Scientific) <i>Fusion for better analytical results in XRF analysis</i></p> <p>14.30 Tea, Exhibition and Posters</p>
<p><b>Tea, Exhibition and Posters</b></p>			

<b>Wednesday 13 April - continued.</b>			
<p><b>CC.00.11: 15.30 – 16.30</b></p> <p><b>In situ Diffraction</b> Chair: Paul Raithby (Bath)</p> <p>15.30 Andy Dent (DIAMOND) <i>In-situ monitoring of oxide-supported metal catalysts by energy dispersive EXAFS, infra-red and mass spectroscopy</i></p> <p>16.00 Simon Redfern (Cambridge) <i>How P modifies high-T disorder in oxides: observations with neutrons</i></p> <p>16.30 Close</p>	<p><b>CC.00.14: 15.00 – 16.00</b></p> <p><b>Crystallography in Industry</b> Chair: Richard Morris (Huntsman Surface Sciences)</p> <p>15.00 Peter Laggner (Graz, Austria) <i>Bridging the nano-gap: simultaneous SAXS and XPD on nanomaterials</i></p> <p>15.40 Ian Cope (Imperial College) <i>Using XRD to support the study of an iron oxide deposit</i></p> <hr style="border-top: 1px dashed black;"/> <p><b>CC.00.14: 16.00 – 16.30</b> <b>AGM: Industrial Group</b> Chair: Jeremy Cockcroft (UCL)</p>	<p><b>CC.00.12/BE.0.25: 15.00 – 16.30</b></p> <p><b>Modern Techniques for Crystal Structure Refinement: CRYSTALS Workshop</b> Organiser: David Watkin, with Richard Cooper, Anna Collins, Stefan Pantos (Oxford)</p> <p>15.00 Brief presentations on several problems relating to refinement, after which participants will be able to use CRYSTALS to try various approaches to solving them. Most of the tools available in CRYSTALS are also available in other programs – the advantage of using CRYSTALS for a workshop is that the tools can be used interactively, with the results displayed graphically.</p> <p>16.30 Close</p>	<p><b>CC.00.13: 15.00 – 16.30</b></p> <p><b>WDXRF Applications and Light Element Analysis.</b> Chair: Margaret West (West X-ray Solutions Ltd)</p> <p>15.00 Rainer Schramm (FLUXANA) <i>Fusion technology for XRF sample preparation</i></p> <p>15.20 Al Martin (RigakuMSC) <i>Light element analysis: the benefits of using a 30 micron tube window for B–O</i></p> <p>15.40 Graham Oliver (CTE, Ceram.) <i>Status of WDXRF in ceramic analysis</i></p> <p>16.10 Close</p>
<p><b>CC.00.11: 16.35 – 17.20</b></p> <p><b>BCA AGM</b> Chair: Chick Wilson (President)</p> <p>17.20 Close</p>			
<p><b>CC.00.11: 17.30 – 18.30</b></p> <p><b>BCA Prize Lecture</b></p> <p>(lecturer to be announced) Chair: Chick Wilson (Glasgow)</p>			
<p><b>19.30 Conference dinner</b></p>			

<b>Thursday 14 April</b>			
<p><b>CC.00.11: 08.30 – 10.00</b>  <b>Phase Transitions Tutorial Session</b>  Organiser: Mike Glazer (Oxford)</p> <p>08.30 Mike Glazer (Oxford)  <i>Critical Aspects of Structural Phase Transitions (tutorial session)</i></p> <p>In this tutorial session a number of topics on structural phase transitions will be introduced, including critical exponents (both in theory and in practice), the Landau theory and its applications, and the role of soft modes at phase transitions. This will be done by reviewing the example of strontium titanate, undoubtedly the most studied and still highly controversial phase transition today. Some class-room demonstrations of critical phenomena and soft modes will be shown. For the purposes of this session little or no basic knowledge of the topic is assumed and therefore this session should be understandable to physical and non-physical crystallographers alike.</p>	<p><b>CC.00.14: 08.30 – 10.00</b>  <b>Non-ambient Pharmaceutical Studies</b>  Chair: Anne Kavanagh (AstraZeneca)</p> <p>08.30 Jonathan Burley (Cambridge)  <i>Crystal structure and intermolecular forces from variable temperature XRPD</i></p> <p>09.00 Jeremy Cockcroft (UCL)  <i>Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies</i></p> <p>09.30 Steve Cosgrove (AstraZeneca)  <i>Probing (de)hydration behaviour by high resolution X-ray powder diffraction</i></p>	<p><b>CC.00.12: 08.30 – 10.00</b>  <b>High Throughput Crystallography</b>  Chair: Jim Naismith (St Andrews)</p> <p>08.30 Michael Sundstrom (SGC)  <i>Directed structural genomics: a protein family approach</i></p> <p>09.00 Keith Wilson (York)  <i>Trying to speed up the 3D structure pipeline: SPINE</i></p> <p>09.30 Stephen Burley (Structural GenomiX, USA)  <i>Structure-guided fragment based drug discovery</i></p>	<p><b>CC.00.13: 08.30 – 10.00</b>  <b>XRF: Standards &amp; Calibration</b>  Chair: Dave Taylor (BCA)</p> <p>08.30 Margaret West (West X-ray Solutions Ltd)  <i>Setting the standards for calibrations</i></p> <p>09.00 Neil Eatherington (British Geological Survey)  <i>An improved analytical methodology using synthetic standards, fused beads and X-ray fluorescence spectrometry for cements and associated materials</i></p> <p>09.30 Ken Field (Oxford Instruments Analytical)  <i>Use of disparate materials for the calibration of anEDXRF spectrometer for the analysis of waste packaging material</i></p>
<b>10.00 Coffee, Exhibition and Posters</b>			
<p><b>CC.00.11: 10.30 – 12.00</b>  <b>Phase Transitions</b>  Chair: Pam Thomas (Warwick)</p> <p>10.30 Jens Kreisel (Grenoble)  <i>Pressure-induced phase transitions in piezoelectric lead-based perovskites</i></p> <p>11.00 Julien Haines (Montpellier)  <i>Stability of the crystal structures of alpha quartz homeotypes at high temperature and at high pressure</i></p>	<p><b>CC.00.14: 10.30 – 12.00</b>  <b>Non-ambient Pharmaceutical Studies</b>  Chair: Roy Copley GlaxoSmithKline)</p> <p>10.30 Francesca Fabbiani (Edinburgh)  <i>Probing polymorphism with high pressure</i></p> <p>11.00 Angus Forster (GlaxoSmithKline)  <i>The use of X-ray diffraction in the pharmaceutical development of a dihydrate API</i></p>	<p><b>CC.00.12: 10.30 – 12.00</b>  <b>High Throughput Crystallography</b>  Chair: Charlie Bond (Dundee)</p> <p>10.30 Samar Hasnain (SRS Daresbury)  <i>Combined X-ray approach for studying metalloproteins function/misfunction: a powerful approach to metallogenomics</i></p> <p>11.00 Bill Duax (Buffalo, USA)  <i>Multiple open reading frames, codon bias and amino acid use and the evolution of the genetic code</i></p>	<p><b>CC.00.13: 10.30 – 12.00</b>  <b>XRF: EDXRF – Applications</b>  Chair: Graham Oliver (CTE Ceram)</p> <p>10.30 Mark Ingham (British Geological Survey)  <i>How does mobile XRFS measure up to contaminated land assessment?</i></p> <p>11.00 Stanislaw Piorek (R&amp;D Niton, LLC)  <i>Field portable XRF for on-site screening and analysis of prohibited substances in plastics</i></p>

<b>Thursday 14 April continued.</b>			
<b>CC.00.11:</b>  11.30 Michael Carpenter (Cambridge) <i>The role of protons in ferroelectric, ferroelastic and coelastic phase transitions in lawsonite, CaAl<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>(OH)<sub>2</sub>.H<sub>2</sub>O</i>	<b>CC.00.14:</b>  11.30 Peter Laggner (Graz, Austria) <i>Monitoring non-ambient nanophase processes by TR-SWAXS</i>	<b>CC.00.12:</b>  11.30 Tom Oldfield (EBI) <i>The MSD relational database</i>	<b>CC.00.13:</b>  11:20 Martin Teasdale (GlaxoSmithKline) <i>EDXRF applications in the pharmaceutical industry</i>  11.40 Simon Fitzgerald (HORIBA Jobin Yvon Ltd) <i>Micro-EDXRF and its applications - non-destructive elemental mapping</i>
<b>12.00 Lunch</b>			
<b>CC.00.11: 13.00 – 14.30</b> <b>Phase Transitions</b> Chair: Kevin Knight (ISIS)  13.00 Laurent Chapon (ISIS) <i>Magnetic phase transitions</i>  13.30 Ivana Evans (Durham) <i>Structural origin of the oxide ion migration pathway in La<sub>2</sub>Mo<sub>2</sub>O<sub>9</sub></i>  14.00 Michael Morris (Cork, Ireland) <i>In-situ studies of order – disorder phenomena in the synthesis of mesoporous silica</i>  14.30 Tea	<b>BE.0.25: 13.00 – 15.00</b> <b>CCP14 Workshop</b> Organisers: Richard Stephenson (UCL), Louis Farrugia (Glasgow)  13.00 This session will start with a WinGX demonstration by Louis Farrugia, followed by a hands-on WinGX workshop  15.00 Tea		<b>CC.00.13: 13.00 – 15.00</b> <b>XRF: Combined XRF/XRD Applications</b> Co-chairs: David Beveridge (Ilford Imaging UK); Dave Taylor (BCA)  13:00 Noel Thomas (WBB Minerals, Germany) <i>Combining XRF, powder XRD and structural modelling techniques: application to plastic clays and kaolins</i>  13.30 Chris Staddon (Nottingham) <i>XRD and XRF studies on GaMnAs thin films</i>  14.00 Discussion  15.00 Tea
<b>Tea and close</b>			