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 12th 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 12th April

Poster Session and Exhibition, with Buffet Dinner and Wine Reception

Wednesday 13 April

CC.00.11: 08.30 – 10.00

In situ Diffraction
Chair: John Evans (Durham)

08.30 Matt Rosseinsky (Liverpool)
In-situ diffraction in inorganic materials discovery and processing

09.00 Poul Norby (Oslo)
In-situ synchrotron studies probing the synthesis/application of inorganic materials

09.30 Roger Davey (UMIST)
Using x-rays for the in situ study of crystallisation processes

CC.00.14: 08.30 – 10.00

Photocrystallograpy
Chair: Paul Raithby (Bath)

08.30 Jacqui Cole (Cambridge)
Single-crystal X-ray diffraction studies of photo-induced molecular species

09.15 Judith Howard (Durham)
Spin cross-over complexes: structures and photomagnetism of high spin, low spin and metastable states and the LIESST effect

CC.00.12: 08.30 – 10.00

At and in the Membrane
Chair: Steve Prince (Manchester)

08.30 Steve Baldwin (Leeds)
Membrane protein expression in the genomic era

09.00 Piet Gros (Utrecht, Netherlands)
Two outer-membrane proteins: translocation through a narrow beta barrel pore and a tilted beta barrel

09.30 Bob Stroud (UCSF, USA)
A two billion year old tale of membrane transport: 'gas' channels and water channels

CC.00.13: 08.30 – 10.00

XRF: Liquid samples.
Chair: David Beveridge (Ilford Imaging UK)

08.30 Siân Shore (Shell Global Solutions)
Overcoming cobalt interference in sulphur analysis

08.50 Al Martin (RigakuMSC)
Ultra carry filter, allowing ppb detection levels by WDXRF

09.10 Gaetan Deshais (BrukerAXS)
Film 2005. A review of thin films used in XRF analysis of liquid samples

09.30 Steve Davis (PANalytical)
Using Activated Alumina for Heavy Metal Contaminants Analysis

10.00 Coffee, Exhibition and Posters

CC.00.11: 10.30 – 12.00

In situ Processing in Industry
Chair: Steve Norval (ICI)

10.30 Gordon Tiddy (Manchester)
Surfactant formulation

11.00 Geoff Moggridge (Cambridge)
Processing block co-polymers for nano-pores

11.30 Simon Jacques (UCL)
In situ crystallisation studies of pharmaceutical materials

12.00 – 12.30 AGM: Chemical Crystallography Group
Chair: Sandy Blake (Nottingham)

CC.00.14: 10.30 – 12.00

Photocrystallography
Co-Chairs: Paul Raithby (Bath); John Helliwell (Manchester)

10.30 Eric Collet (Rennes, France)
The key role of X-ray diffraction for the investigation of photo-induced phase transitions

11.05 Beatrice Vallone (Rome, Italy)
Protein structural dynamics observed by time resolved crystallography

11.40 John Helliwell (Manchester)
The 15K neutron structure of saccharide-free concanavalin A

12.00 Lunch, Exhibition and Posters

CC.00.12: 10.30 – 12.00

Modern Techniques for Crystal Structure Refinement
Chair: Charlie Bond (Dundee)

10.30 Richard Cooper (Oxford)
Advanced techniques in structure refinement

11.00 Thomas Schneider (Milan)
Refinement of proteins as large small molecules using SHELXL

11.30 Garib Murshudov (York):
REFMAC: recent developments towards automatic refinement

12.00 Lunch, Exhibition and Posters

CC.00.13: 10.30 – 12.00

XRF Workshop: Awkward Samples
Chair: David Beveridge (Ilford Imaging UK)

10.30 Awkward samples workshop
An informal session for sharing problems and solutions

12.00 Lunch, Exhibition and Posters

Wednesday 13 April 12.00 Lunch, Exhibition and Posters

CC.00.11: 13.00 – 13.30

AGM: Physical Crystallography Group Chair: Pam Thomas (Warwick)

13.30 – 15.00
In situ Diffraction
Chair: Andrew Harrison (Edinburgh)

13.30 Pam Thomas (Warwick)
Synchrotron X-ray studies of ferroelectrics under applied electric fields

14.00 Mark Smith (Warwick)
The use of in situ diffraction to probe the processing of amorphous silicate-based materials from gelation to reaction with biofluids

14.30 Rudolf Winter (Aberystwyth)
In-situ small angle X-ray scattering study of interface morphology in sintered nano-ceramics

14.45 Amber Thompson (Durham)
In-situ diffraction studies of spin crossover coordination polymers

15.00 Tea, Exhibition and Posters

CC.00.14: 13.00 – 14.30

Crystallography in Industry
Chair: Judith Shackleton (Manchester)

13.00 Michael Preuss (Manchester)
Residual stresses in friction welded aeroengine components

13.30 Tony Fry (National Physical Laboratory)
Residual stress measurements at NPL. Increasing confidence and developing best practice

14.00 Martijn Fransen (PANalytical)
Title TBA

14.30 Tea, Exhibition and Posters

CC.00.12: 13.00 – 14.30

Modern Techniques for Crystal Structure Refinement
Chair: Simon Parsons (Edinburgh)

13.00 Charlie Bond (Dundee):
What's that blob? Identifying metal ions in protein crystal structures

13.30 Bill David (ISIS)
Beyond least squares

14.00 Alan Coelho (ISIS)
TOPAS-Academic, programming ideas

14.30 Tea, Exhibition and Posters

CC.00.12: 14.30 – 14.45

AGM: Biological Structures Group
Chair: Richard Pauptit (AstraZeneca)

14.45 Tea, Exhibition and Posters

CC.00.13: 13.00 – 14.30

WDXRF Applications.
Chair: Mark Ingham (British Geological Survey)

13.00 Margaret West (West X-ray Solutions Ltd)
Keeping it clean

13.30 David Beveridge (Ilford Imaging UK Ltd)
Determination of sulphur and chlorine in organic compounds by XRF

14.00 Michel Davidts (Socachim-XRF Scientific)
Fusion for better analytical results in XRF analysis

14.30 Tea, Exhibition and Posters

Tea, Exhibition and Posters

Wednesday 13 April - continued.

CC.00.11: 15.30 – 16.30

In situ Diffraction
Chair: Paul Raithby (Bath)

15.30 Andy Dent (DIAMOND)
In-situ monitoring of oxide-supported metal catalysts by energy dispersive EXAFS, infra-red and mass spectroscopy

16.00 Simon Redfern (Cambridge)
How P modifies high-T disorder in oxides: observations with neutrons

16.30 Close

CC.00.14: 15.00 – 16.00

Crystallography in Industry
Chair: Richard Morris (Huntsman Surface Sciences)

15.00 Peter Laggner (Graz, Austria)
Bridging the nano-gap: simultaneous SAXS and XPD on nanomaterials

15.40 Ian Cope (Imperial College)
Using XRD to support the study of an iron oxide deposit

CC.00.14: 16.00 – 16.30
AGM: Industrial Group
Chair: Jeremy Cockcroft (UCL)

CC.00.12/BE.0.25: 15.00 – 16.30

Modern Techniques for Crystal Structure Refinement: CRYSTALS Workshop
Organiser: David Watkin, with Richard Cooper, Anna Collins, Stefan Pantos (Oxford)

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.

16.30 Close

CC.00.13: 15.00 – 16.30

WDXRF Applications and Light Element Analysis.
Chair: Margaret West (West X-ray Solutions Ltd)

15.00 Rainer Schramm (FLUXANA)
Fusion technology for XRF sample preparation

15.20 Al Martin (RigakuMSC)
Light element analysis: the benefits of using a 30 micron tube window for B–O

15.40 Graham Oliver (CTE, Ceram.)
Status of WDXRF in ceramic analysis

16.10 Close

CC.00.11: 16.35 – 17.20

BCA AGM Chair: Chick Wilson (President)

17.20 Close

CC.00.11: 17.30 – 18.30

BCA Prize Lecture

(lecturer to be announced) Chair: Chick Wilson (Glasgow)

19.30 Conference dinner

Thursday 14 April

CC.00.11: 08.30 – 10.00
Phase Transitions Tutorial Session
Organiser: Mike Glazer (Oxford)

08.30 Mike Glazer (Oxford)
Critical Aspects of Structural Phase Transitions (tutorial session)

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.

CC.00.14: 08.30 – 10.00
Non-ambient Pharmaceutical Studies
Chair: Anne Kavanagh (AstraZeneca)

08.30 Jonathan Burley (Cambridge)
Crystal structure and intermolecular forces from variable temperature XRPD

09.00 Jeremy Cockcroft (UCL)
Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies

09.30 Steve Cosgrove (AstraZeneca)
Probing (de)hydration behaviour by high resolution X-ray powder diffraction

CC.00.12: 08.30 – 10.00
High Throughput Crystallography
Chair: Jim Naismith (St Andrews)

08.30 Michael Sundstrom (SGC)
Directed structural genomics: a protein family approach

09.00 Keith Wilson (York)
Trying to speed up the 3D structure pipeline: SPINE

09.30 Stephen Burley (Structural GenomiX, USA)
Structure-guided fragment based drug discovery

CC.00.13: 08.30 – 10.00
XRF: Standards & Calibration
Chair: Dave Taylor (BCA)

08.30 Margaret West (West X-ray Solutions Ltd)
Setting the standards for calibrations

09.00 Neil Eatherington (British Geological Survey)
An improved analytical methodology using synthetic standards, fused beads and X-ray fluorescence spectrometry for cements and associated materials

09.30 Ken Field (Oxford Instruments Analytical)
Use of disparate materials for the calibration of anEDXRF spectrometer for the analysis of waste packaging material

10.00 Coffee, Exhibition and Posters

CC.00.11: 10.30 – 12.00
Phase Transitions
Chair: Pam Thomas (Warwick)

10.30 Jens Kreisel (Grenoble)
Pressure-induced phase transitions in piezoelectric lead-based perovskites

11.00 Julien Haines (Montpellier)
Stability of the crystal structures of alpha quartz homeotypes at high temperature and at high pressure

CC.00.14: 10.30 – 12.00
Non-ambient Pharmaceutical Studies
Chair: Roy Copley GlaxoSmithKline)

10.30 Francesca Fabbiani (Edinburgh)
Probing polymorphism with high pressure

11.00 Angus Forster (GlaxoSmithKline)
The use of X-ray diffraction in the pharmaceutical development of a dihydrate API

CC.00.12: 10.30 – 12.00
High Throughput Crystallography
Chair: Charlie Bond (Dundee)

10.30 Samar Hasnain (SRS Daresbury)
Combined X-ray approach for studying metalloproteins function/misfunction: a powerful approach to metallogenomics

11.00 Bill Duax (Buffalo, USA)
Multiple open reading frames, codon bias and amino acid use and the evolution of the genetic code

CC.00.13: 10.30 – 12.00
XRF: EDXRF – Applications
Chair: Graham Oliver (CTE Ceram)

10.30 Mark Ingham (British Geological Survey)
How does mobile XRFS measure up to contaminated land assessment?

11.00 Stanislaw Piorek (R&D Niton, LLC) *Field portable XRF for on-site screening and analysis of prohibited substances in plastics*

Thursday 14 April continued.

CC.00.11:

11.30 Michael Carpenter (Cambridge)
The role of protons in ferroelectric, ferroelastic and coelastic phase transitions in lawsonite, $CaAl_2Si_2O_7(OH)_2.H_2O$

CC.00.14:

11.30 Peter Laggner (Graz, Austria)
Monitoring non-ambient nanophase processes by TR-SWAXS

CC.00.12:

11.30 Tom Oldfield (EBI)
The MSD relational database

CC.00.13:

11:20 Martin Teasdale (GlaxoSmithKline)
EDXRF applications in the pharmaceutical industry

11.40 Simon Fitzgerald (HORIBA Jobin Yvon Ltd)
Micro-EDXRF and its applications - non-destructive elemental mapping

12.00 Lunch

CC.00.11: 13.00 – 14.30
Phase Transitions
Chair: Kevin Knight (ISIS)

13.00 Laurent Chapon (ISIS)
Magnetic phase transitions

13.30 Ivana Evans (Durham)
Structural origin of the oxide ion migration pathway in $La_2Mo_2O_9$

14.00 Michael Morris (Cork, Ireland)
In-situ studies of order – disorder phenomena in the synthesis of mesoporous silica

14.30 Tea

BE.0.25: 13.00 – 15.00
CCP14 Workshop
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

CC.00.13: 13.00 – 15.00
XRF: Combined XRF/XRD Applications
Co-chairs: David Beveridge (Ilford Imaging UK); Dave Taylor (BCA)

13:00 Noel Thomas (WBB Minerals, Germany)
Combining XRF, powder XRD and structural modelling techniques: application to plastic clays and kaolins

13.30 Chris Staddon (Nottingham)
XRD and XRF studies on GaMnAs thin films

14.00 Discussion

15.00 Tea

Tea and close