SCMP @ IoP PCG PCG @ BCA

Newsletter

Spring 2009

FROM THE CHAIRMAN

I am writing this whilst looking out over a very snowy scene in Oxfordshire – it feels anything but spring-like. However, by the time you are reading this the British Crystallographic Association Spring Meeting will be only a month or so away and (hopefully) the weather will be much warmer. As most of you already know, this year the Spring Meeting is being held in Loughborough, 21st-23rd April and various members of the Physical Crystallography - Structural Condensed Matter Physics Group Committee have organised a packed and varied set of sessions loosely based on the overarching conference theme of "Dynamic Crystallography". Please see further details of this, our main annual meeting, later in this Newsletter and if you haven't already done so, register for the meeting at www.crystallography-meetings.org.uk. On the subject of web-sites, the BCA has recently re-vamped its own site, which is now to be found at www.crystallography.org.uk; this includes links to our own wiki-based site at www.pcg-scmp.org.

I am happy to report that our recent SCMP-PCG winter meeting, held in conjunction with the ISIS Crystallography User Meeting at Coseners House Abingdon on 6-7th November 2008, was a big success. We were delighted by the response to this new format meeting, with around 75 participants—easily one of our largest winter meetings—with lively discussion and a friendly atmosphere. We welcome further feedback on the new format for this meeting, and also any general comments about our involvement in the annual Condensed Matter and Materials Physics conference. This is because the CMMP Division of the Institute of Physics have—after a slow yearly decline in attendees—decided to attempt to re-invigorate this meeting, starting with CMMP'09 in Warwick, 15-17th December.

I am told that traditionally the PCG Group has alternated each year between supporting the CMMP conference and holding their own separate winter meeting. This year we plan to hold another winter meeting linked to ISIS Crystallography User Meeting whilst offering limited support of CMMP'09 through the co-sponsorship of a Multiferroics session, jointly with the Magnetism Group. Other CMMP'09 sessions of potential interest to our community include sessions on matter under extreme conditions, strongly correlated systems, energy and nanomagnetism. Please take a look at the full CMMP09 programme (it should be published on the IoP website shortly), consider attending the meeting, and let us have any feedback on how (or indeed whether) we should support this meeting in the future.

I am also very pleased to tell you that Andrew Goodwin, one of our PCG-SCMP members, was awarded the European Powder Diffraction Conference Young Scientist Award at EPDIC-11 in Warsaw last September. More details about this and a brief summary of his prize lecture 'The Crystallography of Flexibility' can be found later in this Newsletter. The meeting itself was well supported by members of our community with plenary lectures given by Andrew and by John Evans (Department of Chemistry, Durham), the latter speaking about negative thermal expansion materials, and several talks from UK participants within the different symposia. One of the other highlights was the conference gala dinner in the building which used to house the communist party headquarters.

For those of you who were inspired by the Satellite Workshop on PDF Methods at last year's BCA Spring Meeting and would like to pursue the techniques of total scattering further, there will be a workshop dedicated to these methods this October in Budapest. 'The First 21 Years of Reverse Monte Carlo Modelling' will be held between 1st and 3rd October 2009 and will be preceded by a two day tutorial workshop. Having been to

previous meetings I am sure that we are guaranteed an informal, quirky event with much helpful discussion. I would particularly like to encourage you to attend in order to increase the representation from those of us who are applying these methods to the study of crystals (and nanocrystals). Please email me if you would like further details about this meeting.

Finally, I would like to thank two Committee members, John Loveday and Serena Margadonna, who have served their full term of office, for their contributions to the activities of the PCG-SCMP Group. As a result, we are seeking nominations for two new Committee members for three years from April 2009.

I look forward to (re)meeting you all in Loughborough in April.

David Keen
PGG-SCMP Chairman

ANNOUNCEMENTS

Vacancies on the PCG-SCMP Committee

Call for Nominations

There are three vacancies arising on the PCG-SCMP Committee: two for the positions of ordinary members and one for the Honorary Secretary/Treasurer. Nominations for these positions are invited and should be sent to the current Honorary Secretary/Treasurer, Matt Tucker (matt.tucker@stfc.ac.uk).

Nominations should include the name of the proposer, the name of the seconder and the nomination acceptance by the nominee, confirming his/her willingness to contribute to the Committee efforts by actively participating in BCA and PCG-SCMP meetings, meeting organisation and our educational activities. Informal enquiries about the Committee members' roles should be directed to the current Chairman (david.keen@stfc.ac.uk).

Elections for these positions will be held at the Annual General Meeting of the PCG-SCMP, which will be held during the BCA Spring Meeting in Loughborough, on Wednesday, 22nd April 2009.

PCG-SCMP bursaries

Student bursary applications are welcome from the BCA or the IoP members affiliated to the PCG-SCMP group. Bursaries are intended to help research students to attend meetings, conferences and training schools relevant to PCG-SCMP areas of interest. Students may apply for up to a total amount of £250 during the course of their PhD.

Applications can be submitted to the IoP throughout the year, but will be considered by the Group Committee on a quarterly basis (and therefore should reach the IoP by 1st March, 1st June, 1st September and 1st December).

Successful bursary applicants are expected to produce a short written report on the meeting, which may be published in this Newsletter (see section Reports from Recent Events in this issue), in Crystallography News or on the PCG-SCMP website (www.pcg-scmp.org).

For further information please contact the PCG-SCMP Honorary Secretary/Treasurer (matt.tucker@stfc.ac.uk) or visit the relevant IoP web page (http://www.iop.org/activity/grants/index.html).

FUTURE EVENTS

Meeting Calendar

- BCA Spring Meeting, 21st – 23rd April 2009, Loughborough
- International Conference on Neutron Scattering ICNS 2009, 3rd – 7th May 2009, Knoxville, Tennessee, USA
- European Materials Research Society Spring Meeting E-MRS Spring 2009, 8 - 13th June 2009, Strasbourg, France
- European Crystallographic Meeting ECM25, 16th – 21st August 2009, Istanbul, Turkey
- Density Functional Methods for Experimental Spectroscopy Workshop, 24 - 28th August 2009, Oxford
- The First 21 Years of Reverse Monte Carlo Modelling, 1st - 3rd October 2009, Budapest
- XVth International Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Condensed Phases, 26 – 29th October 2009, Trieste, Italy
- Condensed Matter and Materials Physics Conference CMMP-09, 15 - 17th December 2009, University of Warwick

BCA Spring Meeting, 21st – 23rd April 2009, Loughborough

The BCA Spring Meeting 2009 is themed "Dynamic Crystallography". The meeting will follow the successful format of recent years and run from 11:30 on Tuesday 21st April to 13:30 on Thursday 23rd April. It will feature a total of 20 scientific sessions, including four PCG symposia.

The PCG Teaching Plenary lecture, entitled *Beyond the Debye-Waller factor*, will be given by Professor Martin Dove (Cambridge) on **Thursday, 23rd April.**

PCG parallel sessions and confirmed speakers include:

Multiferroics (Tuesday 21st April)

John Claridge (Liverpool): *Incommensurate bismuth-based perovskites:* $Bi_2Mn_{4/3}Ni_{2/3}O_6$

Michel Kenzelmann (PSI-ETH): *Title TBC*

Neil Alford (Imperial): *Ferroelectric thin films*

Crystallography Near the Edge (Wednesday 22nd April)

Madeleine Helliwell (Manchester): *Methods and applications of anomalous dispersion in small-molecule crystallography*

Gopinathan Sankar (UCL): *Application of anomalous scattering methods in determining the structure of active sites in complex oxides*

Alison Davenport (Birmingham): *Dynamics of salt films on dissolving metal surfaces*

Hydrogen Storage (Thursday 23rd April)

Neal Skipper (UCL): *Molecular and atomic hydrogen in graphite intercalates*

Martin Jones (Oxford): *Apparatus for simultaneous neutron diffraction and thermogravimetric analysis – the IGA^n*

Andrea Baldi (VU Amsterdam): *Mg-Ti multilayers: nanostructured hydrogen-storage alloys*

Dynamics in Framework Structures (Thursday 23rd April)

Richard Walton (Warwick): *Time-resolved diffraction from flexible metal organic frameworks interacting with guest molecules*

Robert Bell (UCL): *Simulating adsorption phenomena in microporous frameworks*

Ashleigh Fletcher (Strathclyde): *Factors affecting adsorption processes and properties in classical and novel porous materials*

Further details about the conference and the final scientific programme will appear at: www.crystallography-meetings.org.uk

Density Functional Methods for Experimental Spectroscopy Workshop, 24 - 28th August 2009, Oxford

The workshop is targeted towards experimentalists in nuclear magnetic resonance (NMR), vibrational (IR, Raman, INS) and core-level spectroscopy (XANES/EELS) who wish to use density functional methods in their research. It will also be of interest to computational researchers who want to incorporate results from these experimental techniques into their research.

Topics to be covered include:

- Fundamentals of materials modelling
- DFT in the solid state, k-points, Brillouin zones
- Pseudopotentials
- Geometry optimisation
- Introduction to NMR, vibrational and core-level spectroscopies
- Computing NMR properties: EFG, chemical shift, J-coupling (GIPAW)
- Computing vibrational properties
- Computing core-level properties
- Practical aspects of *ab-initio* calculations
- Convergence - how to get accurate results
- Limitations of the calculations, and future perspectives
- Electric field gradient tensors in an amino-acid

The workshop will be comprised of lectures and hands-on tutorials using the CASTEP code. The tutors are a mix of theoreticians involved in the development of computational methods, and experimentalists who have

pioneered the use of simulations in their research. Time will be set aside for participants to discuss their own research projects with the tutors.

The workshop will be based at the Oxford University Department of Materials, with accommodation and evening meals at St Edmund Hall. Participation fee of £100 includes course materials, refreshments and evening meals. For those living outside Oxford, 5 nights bed and breakfast at St Edmund Hall is included in this fee (nights of Sunday 23rd to Thursday 27th August).

Application deadline is 30th April 2009. The application form and further details can be obtained at the workshop web site: http://www.castep.org/workshop09_ad.html.

NEWS

Prizes and awards

EPDIC Young Scientist Prize 2008

Dr Andrew Goodwin from the Department of Earth Sciences, Cambridge was presented with the European Powder Diffraction Conference Young Scientist Award at EPDIC-11 in Warsaw last September. The award, generously sponsored by PANalytical (www.panalytical.com) was presented to Andrew by Martijn Fransen, the XRD Senior Product Manager at PANalytical.

Dr Andrew Goodwin (right) receiving the EPDIC Young Scientist Prize 2008 at EPDIC-11 in Warsaw

Following the presentation, Andrew gave a plenary lecture on the subject 'The crystallography of flexibility: local structure and dynamics in framework materials'. In this talk he summarised how under-constrained bonding within materials can give rise to exotic dynamics which often leads to unusual physical properties such as negative thermal expansion (NTE) and negative linear compressibility (NLC). Throughout his talk he highlighted a number of compounds of interest, many of them containing polyhedral units linked by cyanide 'bridges' and including the colossal thermal expansion material $Ag_3[Co(CN)_6]$, which shows NLC at elevated pressures and NTE that is more than an order of magnitude greater than that displayed by materials such as ZrW_2O_8.

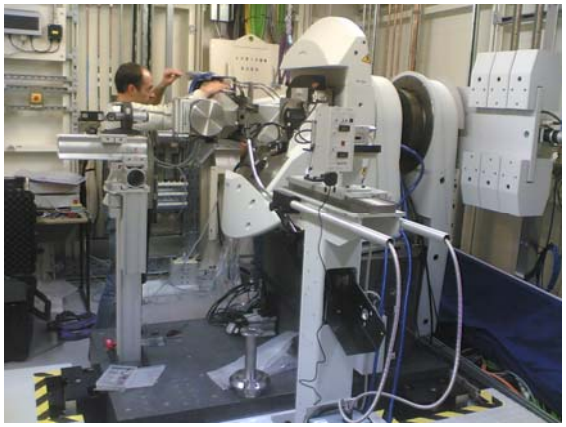
Andrew also outlined some of the methods that he has been developing to probe these materials, including reverse Monte Carlo analysis of total scattering data, a method that he has been using to great effect to reveal the local structure and dynamics from powdered samples. He finished his talk by showing how these techniques can be applied to magnetic systems using the examples of the local magnetic order in spin ices and the spin dynamics in MnO. The talk prompted a lively debate and perfectly set the scene for other talks within the meeting on related subjects where people were also using total scattering methods to understand their particular crystal structure problems.

Beamline News

Diamond Beamline I19: Small-Molecule Single-Crystal Diffraction

The first operational allocation period for the small-molecule single-crystal diffraction beamline (I19) at Diamond has just concluded and, although the beamline construction work has yet to be completed and we are still deep in commissioning, we have supported ten different user groups so far, with a number of these returning for multiple visits. Despite the beamline being in its preliminary stages, and with much commissioning work remaining to fully characterise both the optical components and the diffractometer systems, our initial set of users have had some notable successes. At this early stage, our aims have been fairly modest with the majority of the studies undertaken so far being relatively routine structure determinations, albeit from particularly demanding samples. However, with the recent delivery and installation of the large four-circle diffractometer, which is housed in the second experimental hutch (see photo) we will extend the range of studies the beamline can support to those demanding particularly bulky sample-environment cells. This will hugely increase the scope of work that can be conducted from studies requiring

the very low temperatures (~5 K) provided by a closed-cycle cryostat, those requiring simultaneous high-pressure and variable temperature, and for studies following the time resolution of structural changes following photo-excitation of the sample.



Installation of the large four-circle diffractometer for experimental hutch 2 on I19

The next deadline for beamtime applications via the web pages of the Diamond User Office is imminent, 1st April, for beamtime in the period October 2009 to March 2010. Proposals may be discussed in advance with Dave Allan (david.allan@diamond.ac.uk, Principal Beamline Scientist) or Harriott Nowell (harriott.nowell@diamond.ac.uk, Beamline Scientist) and any particular issues concerning sample preparation can also be discussed with Sarah Barnett (sarah.barnett@diamond.ac.uk, Beamline Support Scientist).

Dave Allan (Diamond)

REPORTS FROM RECENT EVENTS

PCG-SCMP Winter Meeting, 6 - 7th November 2008, The Cosener's House, Abingdon

Whether it was the all-important update of developments at the ISIS second target station or the varied scientific programme focusing on "neutron diffraction and complementary techniques", there was a definite sense of excitement and community at the 2008 PCG-SCMP winter meeting. Held over 6th and 7th November at the Cosener's House, Abingdon, the joint meeting began with a summary of the status and future of crystallography at ISIS. More than 70 UK crystallographers – a healthy mix of students, post-docs, academics and facilities scientists alike – listened as ISIS's Uschi Steigenberger opened the proceedings with a broad update of the ISIS Facility. She reported the successful transfer of beam to TS2 during 2008, and also gave an overview of developments at the existing target station.

Dr Steigenberger was followed by the recently-appointed head of Crystallography at ISIS, Laurent Chapon, who extended this discussion of crystallography instrumentation at ISIS by focusing on the new WISH diffractometer at TS2 and also the POLARIS upgrade at the existing facility. Simon Phillips then introduced a number of the "phase-2" instruments at TS2, while also highlighting new software developments directed at meeting the increasingly varied needs of the ISIS user community (especially with so many new instruments!). He finished with a discussion of the on-site "research hotel" – the nearly-finished Harwell Research Complex – which will reinforce the many strong collaborative links between UK universities and ISIS scientists. Martyn Bull, who runs the communications and media office at ISIS, concluded the User Group meeting with a timely discussion about media outreach and knowledge exchange: he is keen to ensure that both the community as a whole and interested industrial partners are kept informed of the world-class science performed at ISIS.

Scientific discussions (and socialising) during the breaks between sessions

It was, quite literally, a fiery start to the scientific programme as Edinburgh's Colin Pulham described his structural studies of propellants and explosives under extreme temperatures and pressures. A talk for all the senses, with multimedia presentations and even a live demonstration of their explosive power, its scientific highlight was undoubtedly the high-pressure crystallography of the widely-used military explosive RDX (at

pressures up to 80 000 atmospheres, typical of those encountered during detonation). Professor Pulham described how the complementarity of high-pressure x-ray and neutron techniques was needed to determine the molecular rearrangements that distinguish the explosive gamma-RDX form from its more benign ambient phase, alpha-RDX.

Attentive audience in the conference room at the Cosener's House

Very much returning to ambient conditions, Andrew Goodwin from Cambridge then took the floor to describe some recent developments in local-structure techniques aimed at complementing "traditional" diffraction studies of functional materials. Neutron and x-ray pair distribution function methods, density functional theory calculations and electron diffraction were all discussed as tools for understanding local structure/property relationships in some "colossal thermal expansion" cyanides and disordered Bi-containing pyrochlores. Disordered systems were also close to the heart of the following speaker, Steve Hull (ISIS), whose long-standing interest in superionic phases has led him to develop *in-situ* conductivity measurement capabilities at ISIS. His talk, which brought Thursday's proceedings to a close, described the incredibly intricate apparatus involved and detailed some of the preliminary results already obtained using the POLARIS instrument.

The second day of proceedings opened with a broad overview of muSR techniques given by Salford's Sue Kilcoyne. The key focus of her talk was how muon spin relaxation and rotation can help understand internal magnetic fields and spin dynamics in magnetic materials: a probe of local magnetic structure that complements the information obtained from neutron diffraction. The general theme of complementarity was extended to the computational domain by Martin Dove (Cambridge), who gave an overview of techniques for modeling structure and dynamics in crystalline materials. The increased availability of grid-based computing resources and the associated capacity to study materials of enormous complexity were key features of Professor Dove's talk.

PANalytical's support of the crystallographic community is always greatly appreciated, and their funding of the PCG-SCMP Thesis Prize in Physical Crystallography is no exception. The next talk in the proceedings was given by Lars Lundegaard (Edinburgh), the most recent recipient of the prize. It was a fantastic opportunity for all to hear of the science that had earned Lars this award: high-pressure single-crystal x-ray diffraction studies of elemental polymorphs. Deceptively simple in their composition, the elements of Lars's talk – from oxygen to rubidium – showed an incredible variety of complex crystal structures and structural transitions. The practical difficulties of performing diffraction experiments at enormous pressures (up to 100 GPa), and the complexity of the often-incommensurate structures these fundamental materials form under pressure were major obstacles Lars had overcome. His talk left the audience in no doubt that PANalytical had supported a worthy young scientist with a bright future in crystallography!

Lars Lundegaard (Edinburgh) presenting his PANalytical Thesis Prize talk

The final session of the meeting consisted of two talks that were aimed at broadening the experimental palette of the crystallography

community. First was Malcolm Levitt from Southampton, who gave an exceptionally clear presentation on the fundamentals of solid state NMR and the complementary information it could provide when solving crystallographic problems. This was highlighted by his example of solving zeolite crystal structures with magic-angle spinning NMR. Second was Timmy Ramirez-Cuesta (ISIS), whose topical work on hydrogen dynamics in hydrogen-storage candidates formed the basis of the final talk of the scientific programme. Dr Ramirez-Cuesta's complementary technique is that of inelastic neutron scattering, principally using the TOSCA instrument at ISIS.

Dinah Parker (Oxford) receiving her poster prize from the ISIS Crystallography User Group Chairman Phil Lightfoot

At the conference dinner, the poster prize was awarded to Dinah Parker (Inorganic Chemistry, Oxford) for her work entitled "Structure and Magnetic Properties of Compounds Related to the New Superconductor LiFeAs".

It is precisely events such as this that serve to highlight the synergy between crystallography and a broad spectrum of experimental techniques. No doubt the scientific interests of many attendees stand to benefit from the approaches discussed. If as many left the meeting with new ideas as seemed to be the case, then it was a very successful winter meeting indeed.

Andrew Goodwin (Cambridge)

IUCr Congress, 23rd – 31st August 2008, Osaka, Japan

This past August I was tremendously excited to attend for the first time a World Congress of the IUCr, held in the beautiful city of Osaka. The incredibly varied programme, jampacked into nine days, demonstrated that crystallography is on the one hand a mature science, whose methods are applicable to research projects across the spectrum of modern science, and on the other a discipline where fundamental research is still actively expanding frontiers. Indeed, a good deal of the research presented would have been inconceivable only a decade previously. One such session took the study of diffuse scattering to its logical limit of "crystallography without crystals" (that is, diffraction studies on amorphous or even solution-state materials), while another highlighted the rapid development of time-resolved studies such that diffraction measurements on femtosecond timescales are now achievable.

My personal highlight was the keynote lecture by Prof. Masahiro Irie, whose painstaking work on photochromism in diarylethene compounds was both scientifically elegant and aesthetically beautiful. He demonstrated single-crystal-to-single-crystal transformations which could be easily induced or reversed by irradiation with light of an appropriate wavelength. Some materials were co-crystals of several photochromic materials, allowing as many as three different colours to be independently generated at will; others exhibited reversible changes in shape which could be used to kick microscopic "footballs", retaining crystallinity all the while.

My own presentation, on metastable photoisomerism in a family of coordination compounds with potential applications in optical data storage, came at the end of an inspiring afternoon session focussing on the general crystallography of photoexcited states. It seemed to be well received, while nonetheless attracting its fair share of knotty questions!

Other sessions covered topics such as the mathematics behind crystallographic techniques, including the more subtle symmetries needed to describe magnetic ordering or modulated or quasiperiodic materials; computer techniques for solving, refining, storing and indexing crystallographic data; host-guest chemistry of porous crystals, which finds several currently relevant applications including catalysis and hydrogen storage; and diffraction techniques using electrons or neutrons rather than X-rays. Meanwhile, in the hall below, poster presentations vied for punters' attentions with displays advertising central facilities or laboratory equipment, the latter amazingly including a benchtop diffractometer capable of running from an ordinary 240 V wall socket!

I would enthusiastically recommend the IUCr Congresses to anyone with interests in any corner of the diverse field of crystallography – and I for one am already looking forward to the next meeting in Madrid in 2011.

Anthony Phillips (Cambridge)

YOUNG CRYSTALLOGRAPHERS

YC Satellite Meeting, 20-21st April 2009, Loughborough

The Young Crystallographers satellite will be held 20-21st April 2009, prior to the main BCA spring meeting. It will follow the familiar format of sessions starting with a plenary lecture, followed by 15-minute contributed talks.

Further details of the satellite and the full scientific programme can be found at the YC group web pages via: www.crystallography.org.uk.

PCG-SCMP AGM

The 66th PCG-SCMP AMG will take place at the BCA Spring Meeting in Loughborough, on Wednesday, 22nd April 2009, 11:45 – 12:30. Elections for positions of the Honorary Secretary/Treasurer and two ordinary Committee members will be held at the AGM.

The meeting agenda includes the following items:

- Apologies for absence
- Minutes of the 65th PCG-SCMP AGM held in York, 9th April 2008
- Matters arising from minutes
- Chairman's report
- Secretary/Treasurer's report
- Elections to PCG-SCMP Committee
- Future meetings
- Any other business

ACKNOWLEDGEMENT

Many thanks to everyone who contributed to this issue of the PCG-SCMP Newsletter.

Ivana Evans, Durham

PCG-SCMP COMMITTEE

BCA Spring Meeting
21st – 23rd April 2009, Loughborough
"Dynamic Crystallography"

PCG-SCMP Teaching Plenary: Martin Dove
Beyond the Debye-Waller factor

Multiferroics

John Claridge (Liverpool): *Incommensurate bismuth-based perovskites: $Bi_2Mn_{4/3}Ni_{2/3}O_6$*

Michel Kenzelmann (PSI-ETH): *Title TBC*

Neil Alford (Imperial): *Ferroelectric thin films*

Crystallography Near the Edge

Madeleine Helliwell (Manchester): *Methods and applications of anomalous dispersion in small-molecule crystallography*

Gopinathan Sankar (UCL): *Application of anomalous scattering methods in determining the structure of active sites in complex oxides*

Alison Davenport (Birmingham): *Dynamics of salt films on dissolving metal surfaces*

Hydrogen Storage

Neal Skipper (UCL): *Molecular and atomic hydrogen in graphite intercalates*

Martin Jones (Oxford): *Apparatus for simultaneous neutron diffraction and thermogravimetric analysis – the IGA^n*

Andrea Baldi (VU Amsterdam): *Mg-Ti multilayers: nanostructured hydrogen-storage alloys*

Dynamics in Framework Structures

Richard Walton (Warwick): *Time-resolved diffraction from flexible metal organic frameworks interacting with guest molecules*

Robert Bell (UCL): *Simulating adsorption phenomena in microporous frameworks*

Ashleigh Fletcher (Strathclyde): *Factors affecting adsorption processes and properties in classical and novel porous materials*

Further information and registration at: www.crystallography-meetings.org.uk