



FROM THE CHAIRMAN

Welcome to the Physical Crystallography Group-Structural Condensed Matter Physics Group Spring 2010 Newsletter. This Newsletter, as always, contains an interesting mix of reports on past meetings, news from within our community and invitations to future events. I hope that you will enjoy browsing though it.

I cannot really believe that the BCA Spring meeting in Warwick will be starting in less than one month's time! Although term is now over—at least in Oxford—Spring has barely got itself started (indeed someone was commenting to me a couple of weeks ago about how unusual it was that there were no daffodils out for St David's Day; around us in rural Oxfordshire they were still not out for Mothering Sunday) and our thoughts must turn rapidly to the BCA meeting in Warwick. The conference runs from Tuesday 13th until Thursday 15th April and we have planned a typically packed programme of symposia. Full details are contained later in this newsletter and on the BCA meeting website (crystallography.org.uk/bca-spring-meeting-2010) but here I want to congratulate the various PCG Committee members who have co-ordinated sessions containing what I hope will be a stimulating set of talks very vaguely themed about the Conference strap-line of "Data Matters".

In addition to the main meeting, the PCG are also organising a Satellite Workshop on "Local structure, Data Correction Matters" in Warwick and immediately following the meeting (the afternoon of Thurs 15th and the morning of Fri 16th April). This workshop will complement the workshop held two years ago on Pair Distribution Functions and Total Scattering by concentrating on the mechanism of data correction prior to analysis. The workshop is being part-sponsored by ISIS and there may still be a small number of places available. If you are interested then please email our secretary, Matt Tucker (matt.tucker@stfc.ac.uk) for further details.

Our Winter meeting was again held jointly with the ISIS Crystallography User Group Meeting in the very agreeable surroundings of the Coseners House over a couple of days in early November. Around 70 people attended and we heard a series of talks under the title "New results from New Facilities" as well as a talk on hydrogen storage from Martin Jones (Oxford) and on pnictide superconductors from Simon Clarke (also at Oxford) and a number of presentations from students as part of the user group meeting. A full summary of the meeting is contained later in the Newsletter including a number of photographs taken around the bar.

A particular highlight of the winter meeting was the talk from last year's PANalytical sponsored PCG Thesis prize winner, Aurora Cruz-Cabeza. This year we have again received strong applications for the thesis prize, which will be presented to the winner at the BCA spring meeting conference dinner by PANalytical's UK Director, Reg Nicholls. We will also be announcing the 2010 Physical Crystallography Prize at the meeting where the recipient will give a prize lecture.

The reports that I have heard from the Institute of Physics Condensed Matter and Materials Physics Meeting in Warwick just before Christmas were very encouraging with a significant increase in numbers on previous years and a well attended session on multiferroics which we jointly supported. Warwick is clearly a popular place for meetings and CMMP'10 will again be held there this December.

Finally I would like to offer two "thank-you's". First, to Ivana Evans our vice-chair without whom these newsletters would not happen. She co-ordinates, commissions and indeed often writes content and also enables deadlines to be met. Secondly, to our two retiring committee members, Peter Hatton and Andrew Wills, for their valuable work while serving on the committee.

As a result of Peter and Andrew stepping down, I would like to encourage others to consider standing as ordinary committee members at our next election during the

Annual General Meeting at the BCA Spring Meeting in Warwick. If you are interested then please email either Matt Tucker or me or even talk to me at the meeting before the AGM. We would especially like to hear from those within the “physics” wing of Physical Crystallography!

Best wishes

David Keen
PCG-SCMP Group Chair

ANNOUNCEMENTS

Vacancies on the PCG-SCMP Committee

Call for Nominations

There are two ordinary member vacancies arising on the PCG-SCMP Committee. 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 at Warwick University, 13-15th April 2010.

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 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 Institute of Physics web page (<http://www.iop.org/activity/grants/index.html>).

FUTURE EVENTS

Meeting Calendar

- BCA Spring Meeting, 13-15th April 2010, Warwick University
- Powder Diffraction & Rietveld Refinement School, 18th-22nd April 2010, Durham
- Diffraction at the Nanoscale - Nanocrystals, Defective and Amorphous Materials, International Summer School, 24th – 30th May 2010, PSI, Villigen, Switzerland
- Summer School on Mathematical Crystallography, 21st June – 2nd July 2010, Nancy, France
- European Powder Diffraction Conference EPDIC12, 27th – 30th August 2010, Darmstadt, Germany
- European Crystallographic Meeting ECM26, 29th August– 2nd September 2010, Darmstadt, Germany
- Synchrotron Radiation School, 20th – 24th September 2010, Diamond Light Source, Didcot

BCA Spring Meeting, 13–15th April 2010, Warwick University



The BCA Spring Meeting 2010 is themed “Data matters”. The meeting will follow the successful format of recent years and run from 11:30 on Tuesday 13th April to 13:30 on Thursday 15th April.

The PCG Plenary lecture, entitled “Polycrystalline Materials, Powder Diffraction, Electron Microscopy and Charge Flipping – a Remarkable Brew”, will be given by Dr Lynne McCusker (ETH Zurich) on **Wednesday, 14th**

April. PCG parallel sessions and speakers include:

Resonant X-Ray Diffraction (Tuesday 13th April)

Manuel Angst (Julich Forschungszentrum): Title TBC

Paolo Radaelli (University of Oxford): Title TBC

Sean Langridge (ISIS): Title TBC

New Approaches to Structure Solution (Tuesday 13th April)

Sarah Lister (Durham University): *The Use of Complementary Techniques in Structure Solution from Powders*

Maryjane Tremayne (University of Birmingham): *Structure Solution of Multicomponent Systems from Powder Diffraction Data*

Paul Midgley (University of Cambridge): *Towards Routine Structure Solution using Precession Electron Diffraction*

Electron Diffraction (Wednesday 14th April)

Ute Kolb (Johannes Gutenberg-Universität, Mainz): *Enhanced Electron Diffraction Data for "Ab Initio" Structure Solution using Automated Diffraction Tomography*

Sven Hovmöller (Stockholm University): *Single Crystal Diffraction from Powders using Electrons*

Wuzong Zhou (University of St. Andrews): *Electron Diffraction of Some Beam Sensitive Materials*

PDF: Local Structure (Thursday 15th April)

Joseph Hriljac (University of Birmingham): *PDF Studies of the Pressure-Induced Amorphisation of Zeolites*

Daniel P. Shoemaker (University of California): *Local Structure and the Search for Polar Ordering in Geometrically Frustrated Oxides*

Samantha Chong (University of Liverpool): *Investigating Disorder in a Pure Bismuth A Site Perovskite using Total Scattering and RMC Modelling*

PCG Workshop "Local Structure, Data Correction Matters"

The workshop will be held after the main meeting closes at 13:30 on Thursday 15th April.

This workshop will follow on from the PDF and Reverse Monte Carlo analysis workshop held before the York 2008 BCA spring meeting. It will focus on neutron and/or X-ray data collection and data corrections needed for Pair Distribution Function and total scattering analysis. The aim will therefore be to enable people to produce data suitable for the analysis tools demonstrated in the last workshop. If you would like to attend this workshop or would like further information please email the organizer, Matt Tucker (matt.tucker@stfc.ac.uk).

Full details about the conference and the final scientific programme are available at: www.crystallography-meetings.org.uk

NEWS

Prizes and awards

Physical Crystallography Prize 2010

The winner of the 2010 Physical Crystallography Prize will be announced at the BCA Spring Meeting at Warwick. The Prize Lecture will be delivered on Wednesday 14th April.

PANalytical Thesis Prize 2010



The winner of the PANalytical Thesis Prize in Physical Crystallography 2010 will be announced at the conference dinner, at the BCA Spring Meeting at Warwick.

RECENT EVENTS

PCG-SCMP Winter Meeting, 5th - 6th November 2010, The Cosener's House, Abingdon

The PCG-SCMP Winter meeting was held jointly with the ISIS Crystallography User Group Meeting in the Coseners House, Abingdon on Thursday 5th and Friday 6th November 2009. Around 70 people attended the meeting.

The meeting followed the successful format initiated last year starting with crystallography user group business on the Thursday afternoon followed by scientific presentations in the late afternoon and a themed PCG-SCMP session the following morning. There were two scientific talks on Thursday, one from Simon Clarke (Oxford) discussing the work that he has been doing in the structures of layered chalcogenides and the highly topical pnictides and another from Martin Jones (Oxford) describing the work that he has been doing looking at the behaviour of the structures of hydrogen storage materials using in-situ neutron diffraction under various atmospheres. Sandwiched between these talks were a series of short presentations from students and young PDRAs, including the young Mark Weller (Southampton) who was standing in for his PostDoc Valeska Ting who didn't quite make it back from experiments in Australia in time!



The evening session at the PCG-SCMP Winter Meeting 2009 was very popular

The evening was spent perusing a good number of posters, enjoying a drink at the bar (as can be seen from the pictures of Bill David (ISIS) and Simon Clarke) and an excellent dinner during which Stuart Hunter, a PhD student of Duncan Gregory (Glasgow) was presented with a bottled prize for his poster "Towards Nitrogen Transfer Catalysts" by Phil Lightfoot (St Andrew's, ISIS Crystallography User Group Chair and see picture). I understand that conversations and collaborations were then re-established until late into the night...



Phil Lightfoot presenting a bottled prize to Stuart Hunter (Glasgow) for his poster "Towards Nitrogen Transfer Catalysts"

The next day, following a brief introduction from Elspeth Garman (Oxford, British Crystallographic Association President), contained talks from a number of people under the title "New Results from New Facilities". First up was Stephen Moggach (Edinburgh) talking about high-pressure single crystal diffraction on I19 at Diamond. In particular he described some of his work on the unusual compression behaviour of zeolitic imidizolate framework materials (also known as ZIFs) under pressure. Continuing the Diamond theme, Paul Raithby (Bath) talked about his

work on the structures of samples investigated using synchrotron x-ray diffraction while in a photon-induced excited state, which he termed "photocrystallography". The final talk using results from Diamond was by Lucian Pascut (Bristol) who described work using resonant x-ray scattering from I16 to understand the charge ordering in the triangular metallic antiferromagnet AgNiO_2 . There were then two talks describing work from ISIS. The first, by Pascal Manuel (ISIS), showed early results from the WISH diffractometer at the ISIS Second Target Station and the second, by Carlo Vecchini (also ISIS) talked about results from the upgraded HRPD on magnetoelastic coupling from the frustrated antiferromagnetic triangular lattice CuMnO_2 .

In addition to all these talks, we also had an excellent presentation by the 2009 PCG PANalytical sponsored Thesis Prize winner, Aurora Cruz-Cabeza (Cambridge, see picture) who gave a talk on her work investigating the efficacy of methods to predict crystal structures of systems that include more than one molecular type, such as co-crystals, inclusion compounds etc.



Aurora Cruz-Cabeza delivering her PANalytical sponsored Thesis Prize talk at the PCG-SCMP Winter Meeting 2009

All in all the meeting was a great success, with a good balance of different talks from a wide range of systems. Perhaps we'll see you later in 2010 for the next meeting...?

David Keen

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 12th April 2010, Warwick University

The upcoming YCG meeting at the BCA will include talks from Andrew Bond, Andrew Goodwin and Elspeth Garman, as well as a number of presentations from the younger members of the crystallography community.

Also at the YCG meeting, the YCG Annual General Meeting will be held giving Young Crystallographers the opportunity to have their say in the Group activities and vote in new committee members. If you, or anyone you know, would like to get involved in the Young Crystallographers, the posts available are chairperson, vice-chairperson, secretary, CCG representative and IG representative.

Samantha Callear

BEAMLINE NEWS

Wish Starts Successful Operations

Wish, the new magnetic powder and single crystal diffractometer at the ISIS second target station is fully operational and hosted its first external users in December 2009.

A collaborative study between Durham University (UK) and Campinas University (Brazil) used Wish to investigate magnetic structures in Tm_2CoGa_8 and Er_2CoGa_8 at milli-Kelvin temperatures. It is the first instrument in the second target station to achieve these conditions.

PhD student Roger Johnson and MSci student Tom Frawley, both from Durham University, spent time at ISIS to implement the study on the inter-metallic compounds.

The neutron powder patterns Wish provided were of very high quality, despite the samples being experimentally difficult to measure due to their high neutron absorption. Rietveld refinement of the data has enabled the magnetic structure of both compounds to be determined.

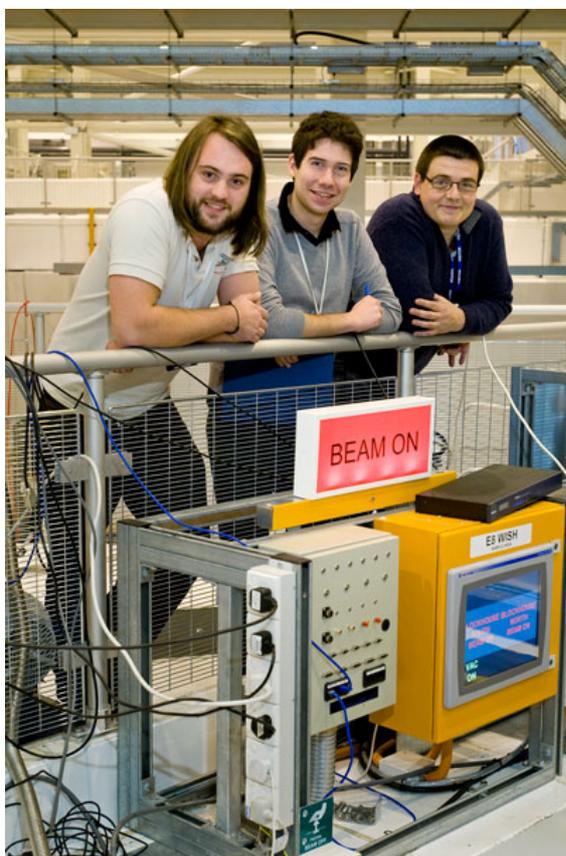
Materials such as these inter-metallic compounds are at the forefront of solid-state research due to a number of them showing novel superconductivity, heavy fermion behaviour and quantum criticality. It is hoped that these findings will make a significant contribution to future understanding of this specific series of materials.

“The understanding of the microscopic behaviour of inter-metallic compounds is very important. Systems that exhibit heavy fermion behaviour and quantum criticality are currently of fundamental scientific interest,” Roger said.

“A microscopic explanation of the magnetic structures measured on Wish may also be transferable to other, more complex systems of technological interest,” he added.

Pascal Manuel, an Instrument Scientist for Wish said, “Everything is running very smoothly, and we hope for a long and successful user schedule to evolve.”

“These results give hints that rapid collection of diffraction patterns on small or absorbing samples in complex sample environments could become routine at ISIS.”



Roger Johnson, Tom Frawley (Durham University) and Pascal Manuel (ISIS) look over Wish whilst it performs its first experiment

Since this first experiment, further successful experiments have been completed and scientific results have been submitted for publication.

Martyn Bull, ISIS

PCG-SCMP AGM

The 68th PCG-SCMP AMG will take place at the BCA Spring Meeting at Warwick University, on Wednesday, 14th April 2010, 11:45 – 12:30. Elections for positions of two ordinary Committee members will be held at the AGM.

The meeting agenda includes the following items:

- Apologies for absence
- Minutes of the 67th PCG-SCMP AGM held in Loughborough, 22nd April 2009
- 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

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BCA Spring Meeting

13th – 15th April 2010, Warwick University
“Data Matters”

PCG-SCMP Plenary: Lynne McCusker (ETH Zurich)

Polycrystalline Materials, Powder Diffraction, Electron Microscopy and Charge Flipping – a Remarkable Brew

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