SCMP @ IoP PCG PCG @ BCA

Newsletter

Autumn 2008

FROM THE CHAIRMAN

Firstly, I want to take this opportunity to say how much I am looking forward to working with the PCG-SCMP Group over the next few years, commitments at home having kept me from the BCA meeting in York in April when I was elected. I also want to thank Paolo Radaelli for his Chairpersonship over the last three years; the Group has been strengthened during his tenure, exemplified by the breadth of well-attended PCG-SCMP meetings, conference sessions and—in particular—the success of the Magnetic Structure Workshop. It is clear that I have a tough act to follow, albeit made much easier by the excellent Committee that I have inherited.

Clearly given the above I can take very little credit for what by all accounts was an extremely successful PCG-SCMP contribution to the BCA Spring Meeting in York this year. I am pleased to report a series of well-attended sessions. Around one hundred people attended "Local structure and disorder in crystalline systems", which followed on from the Satellite Workshop in PDF methods earlier in the week (see Matt Tucker's report for further details). This is an area which is central to much of my own research so I am particularly delighted by the good response to those sessions from the UK crystallographic community. In addition, our joint sessions with the Chemical Crystallography Group on "Crystal Chemistry of Functional Extended Solids" and "Functional Molecular Materials" proved popular. We also had a good number at our two sessions on "Strongly Correlated Electron Systems". Thank you to all who organised and contributed to these sessions. We are already working towards the next Spring Meeting in Loughborough, with Dave Allan and Andrew Goodwin co-ordinating our contributions to this meeting. Please see http://www.crystallography-meetings.org.uk for more details and put the dates in your diaries.

For the first time, the PCG-SCMP Autumn Meeting will take place in conjunction with the ISIS Crystallography User Meeting at Coseners House in Abingdon on the 6th and 7th November 2008. We hope that this arrangement will not only reduce costs for participants but also encourage a wider audience to attend. We have planned the meeting under the title "Neutron Diffraction & Complementary Techniques".

The PCG-SCMP Thesis Prize, sponsored by PANalytical, was won this year by Lars Lundegaard from Edinburgh University and presented to him by Reg Nicholls at the BCA York meeting. We are delighted that PANalytical are continuing to support our Thesis Prize this year and if you would like to nominate yourself or one of your students then please follow the details later in this Newsletter.

I also want to report on exciting developments taking place here at ISIS. The ISIS Second Target Station project has gathered pace over the last six months, culminating in the detection of first neutrons from the TS2 target on the INTER instrument on August 3rd at 13:08. We expect that the WISH diffractometer, also on TS2, will be operational later in the year or early next year. WISH will provide an excellent facility for diffraction experiments from magnetic materials and should be a valuable new resource for our community.

I have just returned from a very enjoyable IUCr Congress in Osaka, Japan where around 2,500 participants had gathered. This meeting showcased the range and quality of work carried out by crystallographers worldwide in many different scientific disciplines. What was also very clear was the strength of the UK contribution within this international community with several UK-based keynote speakers and many invited talks in diverse micro-symposia. It is my hope that the PCG-SCMP group will be able to play its part in promoting UK physical crystallography and physical crystallographers both nationally and internationally for many years to come.

David Keen
PGG-SCMP Chairman

ANNOUNCEMENTS

PANalytical Thesis Prize 2009

Call for Nominations

The Physical Crystallography Group is pleased to invite entries for the PANalytical Thesis Prize in Physical Crystallography. The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a successfully examined thesis submitted in the period from 1st September 2007 to 31st December 2008. The amount of the prize, which will be sponsored by PANalytical Ltd, will be £500.

To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IoP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA/PCG at the student rate to progress their nomination further (current rate £10 per annum or £27.50 for 3 years of the PhD degree).

To enter the competition, candidates must submit:

(a) a copy of the Thesis on CD-ROM.

(b) a personal statement of not more than 500 words explaining why the thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as defined on the website www.pcg-scmp.org or otherwise) in the research.

(c) the names and contact details of two academic referees, one of whom may be the thesis supervisor, who will be able to comment on the thesis research of the candidate.

In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Nominations for the prize must be submitted to the PCG-SCMP Chair, Prof. David Keen (d.a.keen@rl.ac.uk), by 31st January 2009 and the Prize will be awarded at the 2008 BCA Spring Meeting in Loughborough, 21st-23rd April 2009.

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 (m.g.tucker@rl.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 (d.a.keen@rl.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.

FUTURE EVENTS

Meeting Calendar

- 11th European Powder Diffraction Conference (EPDIC), 18-22nd September 2008, Warsaw, Poland
- PCG Autumn Meeting and ISIS Crystallography Users Meeting, 6-7th November 2008, Abingdon
- BCA Spring Meeting, 21st–23rd April 2009, Loughborough

PCG Autumn Meeting, 6-7th November 2008, Cosener's House, Abingdon

PCG Autumn meeting will take place at the Cosener's House, Abingdon, 6-7th November 2009 (lunchtime-to-lunchtime), in conjunction with the ISIS Crystallography Users Meeting.

Registration for the meeting is free. For participants working at UK-based research institutions who attend both meetings or the Users meeting only, the usual allowable travel costs and overnight accommodation will be reimbursed. A limited number of rooms have been pre-booked at the Cosener's House for the meeting. The rooms will be allocated on a first come first served basis.

The meeting is themed "Neutron Diffraction and Complementary Techniques". We have put together a programme of talks which will comprise both an educational element and state-of-the-art science, hoping that the meeting will be of interest to audiences ranging from PhD students to experienced researchers. Confirmed scientific presentations include:

Martin Dove (Cambridge): *Computational Methods in Support of Neutron Scattering*

Steve Hull (ISIS): *Conductivity Measurements in the Neutron Beam*

Sue Kilcoyne (Salford): *Muon Spin Relaxation and Rotation*

Malcolm Levitt (Southampton): *Solid State NMR: A Complementary Technique to Crystallography*

Lars Lundegaard (Edinburgh): *High Pressure X-Ray Diffraction: New Results using Single Crystal Techniques on 'Powder' Diffraction Data*

Timmy Ramirez-Cuesta (ISIS): *Inelastic Neutron Scattering*

Colin Pulham (Edinburgh): *Putting the Squeeze on Energetic Materials – Structural Studies of Propellants and Explosives under Extreme Conditions*

Andrew Goodwin (Cambridge): *When Bragg is Not Enough: "Diffraction Plus" Studies of Framework Materials using PDF, DFT and TEM*

The timetable and online registration are at: http://www.isis.rl.ac.uk/crystallography/usergroup/

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:

- Dynamics in framework structures (organised by Andrew Goodwin and Matt Tucker)
- Hydrogen storage (organised by Dave Keen and Ivana Evans)
- Multiferroics (organised by Andrew Wills and Peter Hatton)
- Crystallography near the edge (organised by Matt Tucker and Dave Allan)

The PCG Plenary lecture will be given by Professor Martin Dove (Cambridge) as the Spring Meeting Teaching Plenary entitled "Beyond the Debye-Waller Factor".

The deadline for abstract submission for poster contributions is 2nd February 2009. Abstracts must be submitted using the template which will be made available on the meeting website.

The scientific programme, further details about the conference and the form for online abstract submission can be found at: www.crystallography-meetings.org.uk

NEWS

Prizes and awards

Physical Crystallography Prize 2008

The IoP-sponsored Physical Crystallography Prize 2008 was awarded to Dr Laurent Chapon, a senior scientist at STFC's ISIS neutron source.

In awarding the prize at the BCA Spring Meeting in York, the PCG-SCMP Chair Professor Paolo Radaelli cited Dr Chapon's outstanding contributions to the development of magnetic neutron diffraction methodology and instrumentation and for its applications as the reason for the award.

"Only a few years ago, magnetic neutron diffraction was considered to be a reactor technique. Laurent's work has been crucial in broadening both the discipline itself and the use of pulsed neutrons," said Professor Radaelli.

Dr Chapon has also developed new software to interpret crystallographic data and make it applicable to pulsed neutrons. This has enabled him to do groundbreaking fundamental work that studies the diverse magnetic properties of materials. His most recent research on multiferroic oxides, which was presented in the Prize lecture, could lead to a variety of applications for the next

generation of electronic devices and data storage.

Dr Chapon is driving future research in this area as project scientist for the new WISH instrument at the Science and Technology Facilities Council's ISIS Second Target Station. By building the instrument he is ensuring that the UK will be at the forefront of this work.

Dr Laurent Chapon receiving his Physical Crystallography Prize 2008 from Professor Paolo Radaelli

"The new instrument will improve magnetic crystallography due to the higher neutron flux at long wavelengths, combined with large detector coverage with good spatial resolution. The WISH instrument will produce clearer data and become the instrument of choice for those using pulsed neutrons for magnetic diffraction," said Dr Chapon.

PANalytical Thesis Prize 2008

The PANalytical Thesis Prize in Physical Crystallography 2008 was awarded to Lars Lundegaard (Edinburgh) for his thesis entitled "High-Pressure Difraction Studies of Rubidium Phase IV".

Rb-IV is unique among the elements in having a composite incommensurate host-guest structure, where the guest chains exist in a ordered or a disordered state depending on pressure. The focus of Lars's PhD work was to refine the full modulated structure of Rb-IV using single-crystal samples and the super-space formalism, resulting in direct information the atomic displacements caused by host guest interactions, which could prove to be the key information that would lead to a better understanding of why this extraordinary phase is stable.

RECENT EVENTS

Powder Diffraction and Rietveld Refinement School, Durham, 14-17th April 2008

The 4th Powder Diffraction and Rietveld Refinement School, generously supported by EPSRC, IUCr, PCG-SCMP, industry and Durham University, ran from Sunday 30th March to Thursday 3rd of April at Van Mildert College and the Chemistry Department at Durham. Lectures were given by Prof Andy Fitch (ESRF), Dr Jeremy Cockcroft (UCL), Dr Ivana Evans (Durham) and Prof John Evans (Durham). Tutorial groups were led by the lecturers and Dr Anne Chippindale (Reading), Dr Lars Peters (Durham) and Miss Sarah Lister (Durham). Miss Julia Payne and Mr David Free acted as tutors during computer practicals.

The School was attended by 60 students from 21 UK Universities and disciplines including Chemistry, Physics, Crystallography, Materials and Engineering, 3 industrial (UK and overseas) and 9 international students from France, Germany, Norway and China.

The School combined lectures, small group tutorials and hands-on computer practicals. Lectures were used to introduce the basic concepts of crystallography, powder diffraction and Rietveld refinement. For each hour of lectures there was at least an hour scheduled for small group problems supervised by tutors to help reinforce the concepts. The remaining ~50% of the course was spent with students going through computer practicals at their own pace. Over 50 computer-based problems were available on a range of different topics, with many containing multiple sub-problems.

Based on the student feedback, we believe that the 2008 Durham Powder Diffraction and Rietveld Refinement School was very successful and that it addressed a key training need. We anticipate running the 5th School at Easter 2010.

John Evans, Durham

BCA Spring Meeting, 8-10th April 2008, York

The BCA Spring Meeting 2008, themed "Structure, Property & Function", was very successful, offering an outstanding scientific programme across diverse areas of crystallography. Over three days, it featured four plenaries, twenty mycrosymposia, prize lecture sessions and it was preceded by an extremely popular hand-on satellite workshop on PDF analysis.

The PCG Plenary lecture "Charge Order in Oxides - Putting the Fun into Functional Materials" was given by Professor Paul Attfield (University of Edinburgh), while parallel sessions covered the following topics: Local Structure and Disorder in Crystalline Materials, Crystal Chemistry of Functional Extended Solids, Functional Molecular Materials and Strongly Correlated Electron Systems.

PCG Poster Prize

There were 22 PCG posters at this year's Spring Meeting poster session and the competition was judged by Thomas Proffen (Los Alamos).

The winner was Sarah Lister (Durham) for her poster entitled "Structures and Phase Transitions in Molybdenum Phosphates". Sarah presented her work on the formation of $(MoO_2)_2P_2O_7$ from a hydrated precursor, which occurs via two previously unknown molybdenum phosphate phases. In order to understand this process, a number of characterisation techniques were used, including *in-situ* variable temperature X-ray diffraction, electron and neutron diffraction and ^{31}P solid state NMR, as well as advanced methodologies for *ab initio* structure solution from powder diffraction data.

The runner-up prize went to Thomas Yip (Strathclyde), for his work on elucidation of structural disorder in garnet-type lithium ion conductors.

Sarah Lister (Durham) receiving the BCA Spring Meeting 2008 PCG Poster Prize from Paolo Radaelli

BCA 2008 Satellite: PDF Workshop, 7-8th April 2008, York

The importance of disorder in crystalline materials is increasingly being recognised as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems. A powerful technique for exploring the local structure of materials is total scattering, also known at the PDF method. Here synchrotron X-ray and/or neutron powder diffraction data are careful corrected and normalised onto an absolute scale, they can then be used to obtain information on the local, medium and long range atomic structure simultaneously. To gain the maximum information from this valuable data specialised refinement methods are required. Two of the most powerful methods currently available for refining this type of data are RMCProfile and PDFGUI.

Working hard at the PDF Satellite Workshop at York

The aim of this workshop was to provide an overview of the methods and the opportunity to gain some hands on experience of applying them to total scattering data. The day began with two one-hour talks by Dr Matt Tucker and Dr Thomas Proffen on RMCProfile and PDFGUI, respectively. This was followed by two one and half hour practical sessions, where participants had the chance to try out the programs by following tutorials and asking questions of Matt, Thomas and Dr Andrew Goodwin. The final one hour session on the morning of the 7th was left as a question and answer session and for people to finish off the exercises.

The workshop was very well attended with about fifty participants taking part; this greatly exceeded our initial estimates and was a very pleasant surprise. During the workshop everyone seemed to enjoy themselves and we

received some very nice feedback following the event. People seemed to particularly like having both methods at the same workshop, so they could compare and contrast what was best for there particular needs and scientific problems. We would like to thank everyone who took part in the workshop and hope you found it as enjoyable and worthwhile experience as we did.

If you would be interested in attending any future workshops on this topic please email Matt Tucker (matt.tucker@stfc.ac.uk) or if you would like to try the methods on your own data please visit our websites (www.isis.rl.ac.uk/RMC or www.diffpy.org).

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 7-8th April 2008, York

It was a very successful meeting by all accounts – over 80 attendees. It was also a successful year for the PCG speakers with Ian Oswald of University of Edinburgh winning the IG prize for best speaker for his talk entitled 'High pressure structures of energetic materials'. Ian's work focuses on detailed structural information on these dangerous but industrially important materials, which can be used to guide development of safer compositions. Other notable speakers were Loretta Lawson's (University of Glasgow) work on magnetic coupling and Graham Stinton (University of Edinburgh) who gave a good overview of the maximum entropy technique and how he has applied it to his work on high pressure nitrogen structures.

We also have three plenary speakers each year, all with a focus on teaching. This year speakers were Ehmke Pohl on macromolecular crystallisation; David Beveridge or the delicacies of the photographic industry and crystallography and David Allan who gave us a fantastic insight into the building of I19 beam line at Diamond and the great array of science that will be accessible using it.

After three years in the role, Simon Coles stepped down as chairman of the YC to be succeeded by Susanne Huth, who was also the first winner of the Durward Cruickshank Young Crystallographers' Prize. Full details of the new committee can be found on our website http://www.chem.gla.ac.uk/yc/index.php. Also on our website you can view the new logo that we have decided to adopt (well at least for a year or so…..).

As you can see from the YC PCG talks, there was once again a strong Scottish biased and this is something that we would love to see changed. If you are a PhD student or an early (2-3 years in) post-doc please get involved. The meeting itself is a great chance to speak or present a poster in a friendly atmosphere. It is also a fantastic opportunity to develop those all-important networking skills. We are still trying to establish our role within the BCA and are keen to hear what you the membership would like in terms of support from the YC. Keep and eye out for possible future winter meetings and involvement with BCA education.

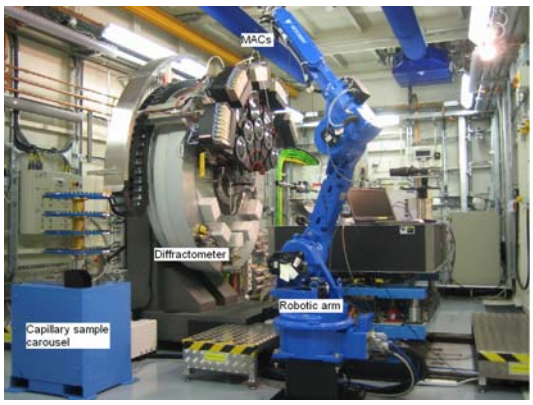
Helen Maynard, Edinburgh

NEWS

Beamline News

Diamond Beamline I11: High-Resolution Powder Diffraction

The high resolution powder diffraction Beamline I11 is the latest Diamond facility to become operational. Beamline Scientists, Chiu Tang, Steve Thompson, Julia Parker and the support team welcomed their first users; a research group led by Dr. Jeremy Cockcroft (University College London) performed a high throughput experiment on this new instrument. They are interested in analysing heat-treated nano-ceramics for better automotive catalyst support materials. The users were helping with the commissioning phase of I11 by testing the efficiency of the beamline's high throughput sample analysis system which includes five banks of MAC detectors (45 Multi-Analysing Crystals and detectors) mounted on the diffractometer, an industrial robot and 200-capillary sample carousel (picture below).



The I11high-resolution powder diffractometer

In addition, the beamline team has systematically commissioned non-ambient cells such as the Cryostream-500 (80 - 500 K), hot-air blower (room temperature - 1000K) and sample tables (small and large). Other sample environments will be commissioned in the next few months, including capillary and flat-plate furnaces and low temperature cryostats (4 - 295 K).

Now the beamline is opened to users, we would like to invite our user community to submit new beamtime applications for the next allocation period, AP5 (Apr – Sep 09). Note the deadline for submission is 1st October 2008.

For more information please visit our website: http://www.diamond.ac.uk/Beamlines/Beamlineplan/I11/default.htm, or contact a member of the beamline staff.

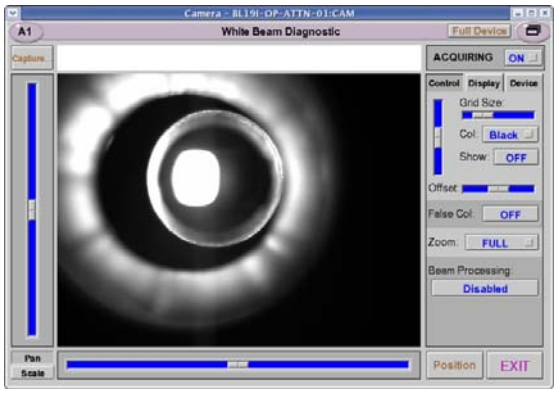
Chiu Tang, Diamond

Diamond Beamline I19: Small-Molecule Single Crystal Diffraction

Commissioning of the small-molecule single crystal diffraction beamline (I19) at Diamond is moving quickly and it is on target to welcome first users later this year in the first of two experimental hutches. The higher throughput of the first experimental hutch will be achieved using a robotic sample changer, which is expected to be ready for use early in 2009.

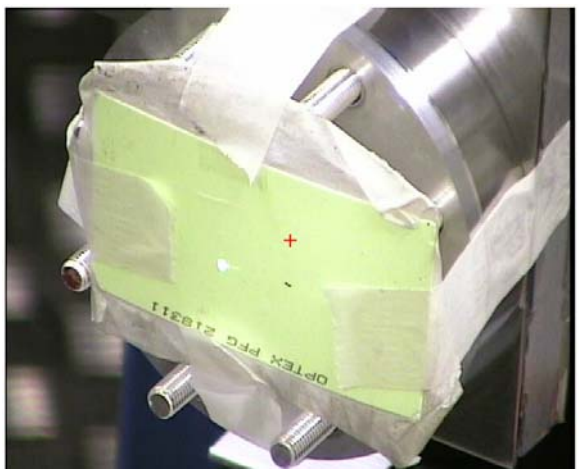
The I19 diffractometer and robotic sample changer housed in experimental hutch 1

The second experimental hutch, which will be available to users from April 2009, will house a larger diffractometer that can support bulkier and heavier sample environment cells, and this hutch will often be used for experiments that require more complex peripheral equipment and longer set-up times.



The white beam from the U21 undulator as it appeared on the first diagnostic element in the optics hutch

First beam into the optics hutch was achieved on 18th June, and subsequently, following successful commissioning of the first two diagnostic units and the primary slits, the monochromatic beam from the double crystal monochromator was observed. Following further commissioning of the monochromator, monochromatic slits, and other diagnostic units, beam has been allowed into the first experimental hutch, and we are looking forward to commissioning the diffractometer with real samples in the next few weeks.



First beam, bright green spot, in experimental hutch 1

The high flux will mean that data can be collected on very small and weakly diffracting crystals, very quickly. Indeed, it is expected that time will be an important parameter in a

large number of the experiments on the beamline; from mapping fast structural changes to characterising short-lived excited states. A wide range of non-ambient conditions will be available to users; pressure experiments will be supported as will variable temperature studies in the range from 4 K, using a cryostat, up to 1300 K, using a gas blower.

The beamline is well equipped for sample preparation with a stereomicroscope for looking at crystals down to 10 μm in size and a high magnification microscope for looking at very small crystals, down to 1 μm, available; both can be equipped with a camera system. Additionally, there is a peripheral laboratory nearby, dedicated to I19 users, which will have wet and dry chemistry areas and facilities which include a second stereomicroscope, crystal manipulation and mounting tools and an oxygen free glove box (N_2) with integrated microscope.

The next deadline for beamtime proposals via the Diamond User Office web pages is 1st October 2008, for beamtime in the period April - September 2009. 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

PCG-SCMP AGM

The PCG-SCMP Annual General Meeting was held during the BCA Spring Meeting in York, on Wednesday, 9th April 2008. Prof. David Keen was elected the Group Chair and Dr. Ivana Evans the Vice-Chair. Dr. Dave Allan, the outgoing Vice-Chair, will remain on the Committee as an Ordinary Member.

The next AMG will take place at the BCA Spring Meeting in Loughborough, on Wednesday, 22nd April 2009. The meeting agenda will be circulated in due course.

ACKNOWLEDGEMENT

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

Ivana Evans, Durham

PCG-SCMP COMMITTEE

PCG-SCMP Autumn Meeting
ISIS Crystallography Users Meeting

"Neutron Diffraction & Complementary Techniques"

6-7th November 2008, Cosener's House, Abingdon

ISIS Facility Update

Crystallography Instrument Review

Scientific Presentations:

Colin Pulham (Edinburgh): *Putting the Squeeze on Energetic Materials – Structural Studies of Propellants and Explosives under Extreme Conditions*

Andrew Goodwin (Cambridge): *When Bragg is Not Enough: "Diffraction Plus" Studies of Framework Materials using PDF, DFT and TEM*

Martin Dove (Cambridge): *Computational Methods in Support of Neutron Scattering*

Steve Hull (ISIS): *Conductivity Measurements in the Neutron Beam*

Sue Kilcoyne (Salford): *Muon Spin Relaxation and Rotation*

Malcolm Levitt (Southampton): *Solid State NMR: A Complementary Technique to Crystallography*

Lars Lundegaard (Edinburgh): *High Pressure X-Ray Diffraction: New Results using Single Crystal Techniques on 'Powder' Diffraction Data*

Timmy Ramirez-Cuesta (ISIS): *Inelastic Neutron Scattering*

Further information at:

www.pcg-scmp.org

http://www.isis.rl.ac.uk/crystallography/usergroup/