



FROM THE CHAIR

Welcome to the Physical Crystallography Group-Structural Condensed Matter Physics Group Autumn 2012 Newsletter! I hope that you'll enjoy browsing through this issue, which contains a mix of meeting reports, information about future events and news from our community.

Since the last Newsletter issue, the most notable event was the BCA Spring Meeting at Warwick, led by the PCG-SCMP Group. I'd like to take this opportunity to thank Kirsten Christensen, who acted as a Chair of the Programme Committee, and the entire programme Committee for putting together an excellent scientific event.

For me personally, the highlight of the Spring Meeting was the PCG Teaching Plenary Lecture entitled "Symmetry modes: Nature's favoured description of structural distortions", given by Professor Branton Campbell (Brigham Young University, USA). I thought, and several student members of the audience to whom I spoke agreed, that Branton offered the clearest ever explanation of those classic undergraduate favourites, irreducible representations and symmetry modes! A full report from Branton's Plenary can be found later in this Newsletter.

We also had an excellent lecture from Dr. Jon Wright (ESRF), winner of the 2012 Physical Crystallography Prize, sponsored by the Institute of Physics.

Speaking of prizes, we again had excellent nominations for the PANalytical Thesis Prize competition. The prize was awarded to Dr. Lucian Pascut for his thesis entitled "Neutron and Resonant X-ray Scattering Studies of Low Dimensional Quantum Magnets", defended at the School of Physics, Bristol University. We are very grateful to PANalytical for continuing to sponsor the Thesis Prize.

Looking ahead to future events, our Winter Meeting this year will keep the successful and popular format of the last few years, and will be held in conjunction with the ISIS Crystallography User Group Meeting, at the Cosener's House, Abingdon, 8-9th November 2012. As in previous years, the meeting will be

supported by ISIS Crystallography Group and the Institute of Physics. The programme is currently being developed, but will be advertised in due course at: <http://www.pcg-scmp.org/Meetings/Winter2012>, where you will also be able to find a link to the online registration form. I hope you will be able to join us for what has become a very successful, intensive two-day meeting.

Next year will be slightly unusual, in that there will be no BCA Spring Meeting. The reason for this is that the UK will host the European Crystallographic Association Meeting (ECM28), which will be held at Warwick, 25-29th August 2013. All information about the programme, registration and abstract submission will appear in due course at the meeting website, <http://ecm28.org/>.

However, in 2013 we will nevertheless be awarding the PANalytical Thesis Prize. The calls for nomination can be found in this Newsletter.

Ivana Evans
PGG-SCMP Chair

ANNOUNCEMENTS

PANalytical Thesis Prize 2013

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 2011 to 31st December 2012.

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.

To enter the competition, candidates must submit:

- (a) a copy of the thesis in electronic format.
- (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, Dr. Ivana Evans (ivana.radosavljevic@durham.ac.uk), by 31st January 2013. The winner will be announced in the spring 2013, but the prize will be formally awarded at the PCG-SCMP Winter Meeting 2013.

Bursaries

The PCG-SCMP members are eligible to apply for bursaries to enable or help them attend scientific conferences. Applications are made to the main organisation to which the young scientist belongs (the BCA or the IoP).

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).

For more information and application forms, please visit the relevant web pages of your main organisation:

<http://crystallography.org.uk/bursary>

http://www.iop.org/about/grants/research_student/page_38808.html

Successful bursary applicants are expected to produce a short written report on the meeting, which may be published on this web site, in the PCG-SCMP Newsletter and/or the Crystallography News.

EDUCATION

The PCG now has a web page devoted to crystallographic education at <http://www.pcg-scmp.org/Education>. On this page I have added a number of references to existing websites where you can find several items of interest, including topic devoted to general crystallography, dynamics, symmetry, diffraction and refinement. At the present time there are 18 links to external sites which I hope you find useful and interesting. It would be helpful if you could contact me with any other websites that we could usefully add.

Mike Glazer (University of Oxford)

FUTURE EVENTS

PCG-SCMP Winter Meeting 2012, 8-9th November 2012

Will be held at Cosners house. Please see the group website (<http://www.pcg-scmp.org/Meetings>) where details on the program and information on registration will soon be hosted.

BCA/CCG Intensive Teaching School in X-ray structural analysis. 6th-14th April 2012

Registration is now open for the 14th BCA/CCG Intensive Teaching School in X-ray Structure Analysis which will run from the 6th-14th of April 2013 in Durham. The school is intended primarily for younger scientists with some experience of structural analysis who wish to improve their understanding of the underlying principles and practice.

<http://www.dur.ac.uk/durham.x-ray-school/>

ECM28 25-29th August 2013

ECM28 will be held in the UK at the University of Warwick. There is current call for suggestions of satellite meetings, please see the website (www.ecm28.org) for more details.

International conference on Neutron Scattering (ICNS) 8-12th July 2013

The next International Conference on Neutron Scattering will take place in Edinburgh, at the Edinburgh International Conference Centre, from 8 - 12 July 2013. ICNS 2013 will bring together scientists from a wide range of disciplines including biology, chemistry, earth science, engineering, materials science and physics.

<http://www.icns2013.org/home>

NEWS

Prizes and awards

2012 Physical Crystallography

This year's prize was won by Dr Jon Wright, ESRF for his work on the Verwey transition of magnetite.



PCG Physical Crystallography prize winner Jon Wright giving his prize lecture with PCG chair, Dr Ivana Evans, looking on.

PANalytical Thesis Prize 2012

The 2012 PANalytical thesis prize was awarded to Lucian Pascut of the School of Physics, University of Bristol. In his own word's Lucian described his prize-winning research:

Many properties of technologically-important materials, such as superconductivity, colossal magneto-resistance and multiferroic effects, metal-insulator transitions, etc. are consequences of the strong electron correlations which lead to cooperative behaviour of the electrons. The fact that this behaviour cannot be easily anticipated from the local interactions among the electrons makes strongly-correlated electron systems a research field at the very forefront of condensed matter research, with a large potential to discover novel forms of electronic order. The subject of my thesis is the investigation of electronic order and dynamics in three different correlated electron systems using synchrotron resonant X-ray and neutron scattering techniques. The main project of my thesis was to probe experimentally the theoretically predicted spontaneous charge order in the orbitally degenerate triangular metal AgNiO_2 . Using single crystal x-ray resonant scattering measurements I developed a complex strategy/data analysis to empirically extract the anomalous contribution to atomic scattering factors, which provided information about the "electronic configuration" at the Ni sites. The large energy difference of 2.5 eV in the anomalous scattering factors (which we understood in detail using band structure calculations in the LDA approximation), is consistent with the predicted charge disproportionation at the Ni sites. The second

project of my thesis involved understanding from the theoretical point of view, the strong anisotropic effects in the Ising magnet CoNb_2O_6 and compare the predicted transitions between energy levels with those observed via inelastic neutron scattering. A good agreement was obtained between the calculated and experimentally measured transition energy levels, direction of the easy-axis, the absolute value of the magnetic moment and the g-tensor. In the last project of my thesis I used elastic and inelastic neutron scattering to probe experimentally changes to the magnetic structure and collective spin fluctuations as a function of magnetic field, upon crossing the critical point in the quantum easy-plane magnet Cs_2CoCl_4 .

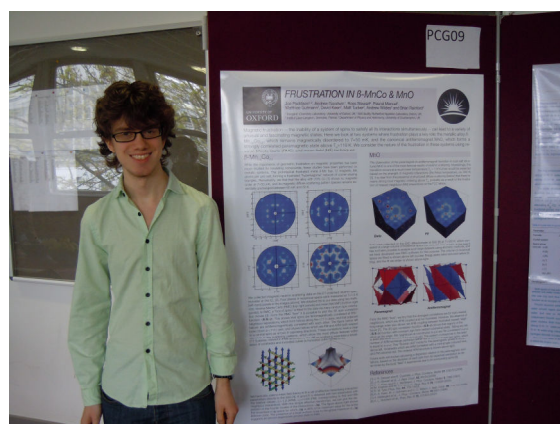
I would not have been able to achieve all this without having the scholarship that I received from the Bristol University and Harold Herbert Potter Fund for which I am very grateful. I would also like to take advantage of this opportunity to express my deepest gratitude to my supervisor Dr. Radu Coldea who has provided me with constant support and encouragement during my PhD and after...



Winner of the 2012 PCG/PANalytical thesis prize – Lucian Pascut.

PCG poster prize

Joe Paddison of Oxford University won this year's PCG poster prize with work entitled 'Frustration in $\beta\text{-MnCo}$ and MnO .'



Joe Paddison and his prize winning poster.

Other news

Former PCG Chair elected president of the BCA

The PCG is proud to report that our former chair, Prof David Keen, has been elected president of the BCA.

International Year of Crystallography



On 3 July at its Sixty-Sixth General Assembly, the UN officially adopted a resolution that 2014 should be the International Year of Crystallography.

The International Union of Crystallography will mark the centennial of the birth of modern crystallography during this year (IYCr 2014). The worldwide crystallographic community has enthusiastically welcomed the idea of having 2014 as an International Year of Crystallography and the Regional Associates and several National organizations have already started their preparations in eager anticipation of the IYCr.

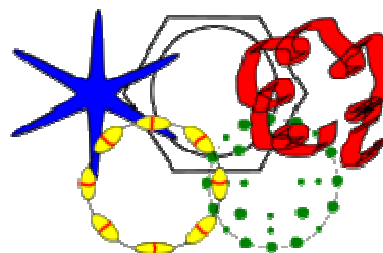
Missing minutes

Do you know the whereabouts of the historical minute book of the "X-ray Analysis Group" now known as the "Physical Crystallography Group"? All minutes from the first committee meetings when Bragg was chair up until ~1990, were pasted into a leather bound book. All the documentation belonging to the Group were kept in a filing cabinet in the basement of 67 Belgrave Square (the previous IOP premises), including the minute book.

Previous secretaries to the Group have been contacted and the IOP archive has been searched, but to no avail. The book is ~100 mm thick and >A4 size, so it is quite distinctive! This has some historical interest and the BCA are interested in its whereabouts. If you have any information, ideas or clues then please can you contact the BCA President or a member of Council.

RECENT EVENTS

BCA Spring meeting 16th-19th April 2012, University of Warwick



The theme and logo of the 2012 BCA spring meeting was chosen in the light of the UK's hosting of the Olympic Games. During the meeting the PCG sponsored or co-sponsored six sessions, as well as awarding this year's teaching plenary and the PCG prize talk.

PCG-SCP Teaching Plenary 2012

The Teaching Plenary Lecture at the BCA Spring Meeting 2012 was given by Professor Branton Campbell (Department of Physics and Astronomy, Brigham Young University, USA), and entitled "Symmetry modes: Nature's favoured description of structural distortions".

Branton's lecture focussed on how the symmetry modes of a distortion (the active basis functions of the irreducible representations of the parent symmetry group) can be used to describe phase transitions, by providing a set of structural parameters, distinct from, but equivalent to the traditional crystallographic parameter set (atomic xyz coordinates), with many intrinsic advantages. Because phase transitions tend to break the parent structure symmetry in a very specific way, symmetry-motivated parameters allow one to distinguish a relatively small number of structural parameters that are active in a particular distortion, from those that are not. In this sense, the symmetry-mode description is far more "natural".

Branton and colleagues at Brigham Young University develop ISODISTORT software, which allows one to simultaneously employ symmetry modes involving atomic displacements, lattice strains, magnetic moments, occupancy orderings and even rigid-body rotations, at both commensurate and incommensurate wave vectors. This was initially described in: B.J. Campbell, H.T. Stokes, D.E. Tanner and D.M. Hatch (2006), *J. Appl. Cryst.* 39, 607-614.; H.T. Stokes, B.J. Campbell and D.M. Hatch (2007), *Acta Cryst.* A63, 365-373. Recent advances and applications include the direct refinement of symmetry-mode amplitudes and the structure determination and symmetry-detection of a distorted structure from powder diffraction data (B.J. Campbell, J.S.O. Evans, F. Perselli and H.T. Stokes (2007), *IUCr Comp. Comm. News*, 8, 81-95; S. Kerman, B.J. Campbell, K.K.

Satyavarapu, H.T. Stokes, F. Perselli and J.S.O. Evans (2012), *Acta Cryst.* A68.

Ivana Evans (Durham University)

Phase Transitions I: Distortion Mode Analysis

The aim of this session, chaired by Ivana Evans, was to follow on from the PCG-SCMP Teaching Plenary, and provide a link between fundamentals of symmetry mode analysis and the topical materials research and state-of-the-art diffraction data analysis.

The first speaker was John Evans (Durham University), whose talk was entitled "Symmetry Mode Analysis of Functional Materials". John gave a number of examples of the direct Rietveld refinement of mode amplitudes, which enabled understanding of a range of structural solid state chemistry problems, including displacive phase transitions in framework materials, cation site ordering in transition metal oxochalcogenides, and magnetic refinements.

The second talk, entitled "The Verwey Structure of Magnetite: Charge Order and Three-Site Distortions" was given by Mark Senn (University of Edinburgh). The mineral magnetite (Fe_3O_4) undergoes a complex structural distortion and becomes electrically insulating below 125 K. Mark described the low temperature structure of magnetite, obtained by high energy x-ray diffraction using an almost single domain 40 μm grain. This structure can be described by a superposition of 168 atomic displacement waves (frozen phonon modes). The observed anomalous shortening of some Fe-Fe distances indicates that the localised electrons are distributed over three-atom 'trimeron' units, now thought to be significant quasiparticles in magnetite above the Verwey transition, and in other spinels.

The final speaker in this session was Phil Lightfoot (University of St. Andrews), with a talk on "New Twists on the Perovskite Theme: the Elusive Phases R and S of NaNbO_3 ". Sodium niobate, NaNbO_3 , has previously been described as 'the most complex perovskite ferroelectric known', having at least seven phases as a function of temperature. Despite more than 40 years of study, the structures of phases R (360 – 480 °C) and S (480 – 520 °C) have not been convincingly elucidated. Phil described new models for both phases, using a combination of the best quality powder diffraction data and a systematic approach using symmetry mode analysis via ISODISTORT software.

Ivana Evans (Durham University)

Hydrogen-bonding: From Water to Supermolecules (Part 1)



Speakers and chair of the hydrogen-bonding session (l to r) Ben Murray, Angelos Michaelides, Dominic Fortes and Christophe Saltzmann.

This session was part of a double session jointly organised by the PCG and CCG to highlight the importance of the phenomenon of hydrogen bonding for crystallography. The PCG session focused mainly on hydrogen bonding between water molecules, and the topic was approached from the experimental as well as theoretical side.

The first talk by Dr Ben Murray (University of Leeds) was entitled "The Structure of Ice Crystallised from Supercooled Water" and showed that a metastable phase of ice, which has previously been called cubic ice, should in fact be named stacking-disordered ice in order to emphasise the fact that this phase contains considerable amounts of hexagonal stacking faults. The implications of the stacking disorder for ice under atmospherically relevant conditions were discussed.

Prof. Angelos Michaelides (University College London) spoke about the "Quantum Nature of the Hydrogen Bond". His talk reported on new insights into the effect of the quantum nature of the hydrogen atoms on the strength and length of hydrogen bonds.

"More Ice than Salt – New Observations of M^{2+}XO_4 cryohydrates" was the title of the last talk in this session given by Dr Dominic Fortes (University College London). A variety of binary phase diagrams of salts and ice were explored, and several new water-rich hydrates were discovered. The importance of those phases in planetary geology was discussed.

Christophe Saltzmann
(University College London)

Piecing Together the Puzzle – Multidimensional Approaches (CCG, YCG & PCG)

Lynne Thomas (Bath) kicked off this session jointly organized by the CCG, YCG and PCG. She gave a presentation entitled 'Beyond the Structure: Investigating Properties in Molecular Materials.' She spoke about the approaches she'd taken to investigate the structural chemistry of target drug molecules for example, in order to improve their physical properties. One particular way of doing this is with co-crystallisation. Crystal engineering can be used to match hydrogen bond donors and acceptors with the addition of a second 'template' molecule. She then moved on to talk about experiments she had carried out with both X-ray and neutron sources, and also materials she had studied with diffuse scattering to help gain a better understanding of why materials behave in a certain way.

Andrew Goodwin (Oxford) then went on to talk about 'Frameworks, Flexibility and Frustration.' He spoke about how framework materials can be designed and constructed with a degree of flexibility within them; this can lead to interesting crystal dynamics. In particular he spoke about framework materials that behaved in a similar way to a foldable wine rack when temperature and pressure were applied to the sample. It was possible to reversibly convert between different phases of the materials, without any loss in crystal quality.

The session was concluded by two talks from Young Crystallographers, Mark Eddleston (Cambridge) and Christopher Woodall (Bath). Mark talked about using transmission electron microscopy combined with crystal structure prediction to help in structure determination. The combination of these two techniques allowed the solution of structures from very small samples, which would otherwise be impossible with conventional single crystal diffraction. The technique requires just a few experimental electron diffraction images, which are used to identify the corresponding crystal structure from a calculated set of low energy crystal structures.

Chris completed the session with a presentation entitled 'An Investigation in the Luminescent Behaviour of Gold(I) Trimers at Variable Temperature and Pressure.' He spoke about a number of Gold(I) complexes he had synthesised and studied at a number of different pressures and temperatures. The compounds underwent a number of phase transitions, and Chris has been studying them to understand the unusual phase transitions that he had been observing!

Anna Warren (Diamond Light Source)

ACKNOWLEDGEMENT

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

Helen Maynard-Casely
(Australian Synchrotron)

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