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Newsletter

Spring 2013

FROM THE CHAIR

Welcome to the Physical Crystallography Group-Structural Condensed Matter Physics Group Spring Newsletter 2013 – the year of the Bragg Centenary!

The 2013 Spring Newsletter is reaching you a bit later than usual, although that's got nothing to do with the weather – the very late spring this year, but with another anomaly: the absence of the BCA Spring Meeting.

As you're probably aware, this is due to the UK hosting the 28th Meeting of the European Crystallographic Association, ECM28, which will be held at the University of Warwick, 25–29th August 2013**.** Further details about the programme and the relevant deadlines can be found in the Newsletter.

In November 2012, we held the PCG-SCMP Winter Meeting in what is becoming our traditional and successful format, with the meeting being held over two days, jointly with the ISIS Crystallography Users' Meeting.

You may remember that at the last AGM I announced the plan to update the group Constitution, last revised in 1985. This was carried out in consultation with the IoP and the BCA, and the new Constitution was approved by both institutions last autumn. Finally, at the Winter Meeting 2012, there was an Extraordinary General Meeting, at which we formally adopted the new group Constitution. The Constitution has been posted on the PCG-SCMP wiki site.

This year's PANalytical Thesis Prize saw, in my opinion, one of the best competitions we've had since I joined the Committee. The standard of all theses entered was truly excellent. In the end, the Committee vote decided to award the 2013 PANalytical Thesis Prize to Mark Senn (Edinburgh), for his PhD thesis entitled "Charge, orbital and magnetic ordering in transition metal oxides".

One of the key aspects of Mark's PhD work focussed on the structure of magnetite below the Verwey transition. This is a very complex structure, adopted by a chemically simple compound, Fe_3O_4. Magnetite is a mineral which can be found in many locations on the Earth. Below is a photo of a sample found in the Smithsonian Museum of Natural History in Washington, D.C., showing a smiling Jon Wright (ESRF), one of Mark's collaborators on this project, posing happily, oblivious to the serious scientific discussion taking place behind him (which, if I remember correctly, was about the colour centres in fluorite).

Jon Wright and magnetite at the Smithsonian Museum of Natural History

I would like to thank PANalytical for their generous continued support of the Thesis Prize, and also to encourage supervisors to continue to nominate outstanding recent PhD graduates for this prize. The next call for nominations will be issued later this year in the Autumn Newsletter and on the group wiki site.

There have been a few recent changes on the PCG-SCMP Committee. Firstly, I'd like to thank two retiring members, Kirsten Christensen and Helen Maynard-Caseley, for their contributions over the last few years, and to wish them all the best in their future endeavours. I'd also like to welcome two new Committee members: Emma McCabe (Kent) and Matthias Gutmann (ISIS).

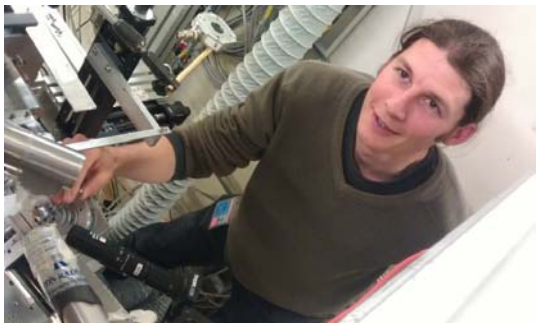
2013 is the year in which we celebrate the Bragg Centenary. Many BCA members have been contributing to the events marking the centenary, including the PCG-SCMP Education Officer, Professor Mike Glazer. Mike is also leading the organisation of a major exhibition entitled "The Two Braggs", which will take place during the ECM28 at Warwick. More details about both events can be found in this Newsletter, which I hope you enjoy!

Ivana Evans (PGG-SCMP Chair)

ANNOUNCEMENTS

PANalytical Thesis Prize 2013

The PANalytical Thesis Prize 2013 has been awarded to Mark Senn (School of Chemistry and Centre for Science at Extreme Conditions at the University of Edinburgh), for his PhD thesis entitled "Charge, orbital and magnetic ordering in transition metal oxides".



Mark Senn, winner of the PANalytical Thesis Prize 2013

Here is a description of his thesis in his own words:

'I have used both single crystal and powder diffraction data collected at central facilities in Grenoble and those located at the Rutherford Appleton laboratory to probe the structure-property relationship in a variety of transition metal oxides.

The focus of my PhD was been that of the low temperature structure of magnetite (Fe_3O_4) which is linked to the well know metal to insulator phase transition that occurs at ~125 K (The Verwey transition) and has long been cited as the first example of charge ordering. The extremely complex nature of the low temperature structure, severe crystal twinning and presence of multiple scattering makes the crystallography very challenging and for this reason the structure has remained unsolved for over 70 years. With help from Jon Wright at ID11, ESRF we performed a highly precise single crystal diffraction study of this structure using a grain of magnetite no large than 20 µm. Our approach has been to reduce the amount of twinning through experimental methods, and use group theory to correctly model any residual twin domains. I have analysed the structure which has 168 internal degrees in terms of the local coordination environments such as the $Fe^{2.5+}O_6$ octahedra and in terms of the normal lattice modes. Our results confirm the presence of charge ordering at low temperatures in magnetite explaining why it undergoes a metal to insulator transition. However, we have discovered that the charge ordering is only stabilised by a novel three-site orbital interaction of two Fe^{3+} and one Fe^{2+}. These three-site interactions account for the large off-centre distortions in the crystal structure of magnetite below the Verwey transition explaining why it is also a ferroelectric material. This observation provides us with a novel mechanism to realise new multiferroic materials in transition metal oxides.'

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 instructions, please visit the relevant web pages of your main organisation:

http://crystallography.org.uk/bursary

or

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

Successful bursary applicants are expected to produce a short written report on the meeting, which may be published in the PCG-SCMP Newsletter.

FUTURE MEETINGS

European Crystallographic Meeting 25th–29th August 2013

Registration for the 28th Meeting of the European Crystallographic Association is now open. ECM28 will be held in the UK at the University of Warwick, 25–29 August 2013**.**

The program of the meeting can be viewed at:

http://ecm28.ecanews.org/programme/

ECM28 Satellite Meetings

There are a number of satellite meetings and symposiums of ECM28 that may be of interest to PCG-SCMP members**.**

Local Structure of Crystalline Materials Using PDF Analysis, 30th–31st August 2013

The aim of this workshop is provide an introduction to total scattering/PDF analysis of crystalline materials.

The topics covered will include: how to collect the diffraction data, how to produce the corrected total scattering and how to model the data and extract the useful information. It is hoped the final programme will be modified to meet the needs of the workshop participants.

The workshop will be held over two full days starting in the morning of the 30th August after the main ECM meeting. The registration fee (including tea, coffee and lunch on both days and possibly dinner on the 30th August if it fits in the cost) is currently planned to be €125.

Registration (including accommodation bookings not included in the registration fee) will be via the ECM28 website.

Further details will be posted on the PCG-SCMP wiki as they become available.

http://www.pcg-scmp.org/Meetings/PDFworkshops2013

European Young Crystallographers Satellite Meeting, 25th August

The European Young Crystallographers Satellite Meeting will take place at ECM28, Warwick, UK on Sunday 25th August 2013. This satellite meeting will be the first of its kind at a European level and will run from 9.00 am to 5.00 pm, with three sessions dedicated to young crystallographers (anyone under the age of 35) presenting their work.

This meeting is organised by the European Young Crystallographers' General Interest Group and the Young Crystallographers' Group of the British Crystallographic Association, in order to promote interaction between up-and-coming and more established crystallographers. We feel that this satellite meeting is an extremely valuable event for young researchers and believe that it will help create a network for young crystallographers, enabling them to communicate their research in an informal environment and to establish connections with other young crystallographers. Given the significance of 2013 to many crystallographers around the world with the Bragg centenary, we want to ensure that we celebrate the contributions of younger members and to continue promoting the fantastic work of these up-and-coming scientists.

A Special Symposium to Mark the Bragg Centenary 26th August

The ECM28 will host a special symposium organised by the Bragg Lecture Fund Committee to mark the Bragg Centenary, on 26th August 2013.

The Bragg Lectures are usually awarded by the committee every three years, but to mark this special anniversary, three lectures have been awarded for a symposium at the ECM 28 meeting in Warwick in 2013; these are: Prof. John Jenkin, biographer of William and Lawrence Bragg (La Trobe University, Australia), Dr. Airlie McCoy, (University of Cambridge), and Prof. Bill David (ISIS Facility RAL and University of Oxford).

NEWS

Powder Diffraction on Mars

Members may also be interested in the milestone reported by NASA late last year, the first diffraction pattern collected on another planet. Collected on the 'Curiosity' rover's CheMin instrument, a suitcase-sized powder diffraction and fluorescence instrument sent along with nine other instruments to the red planet.

The specific sample for CheMin's first analysis was soil Curiosity scooped up at a patch of dust and sand that the team named Rocknest. The sample was processed through a sieve to exclude particles larger than 0.006 inch (150 micrometers), roughly the width of a human hair. The sample has at least two components: dust distributed globally in dust storms and fine sand originating more locally.

http://www.jpl.nasa.gov/news/news.php?release=2012-341#7

EDUCATION

Celebrating Crystallography
Bragg Centenary 1913 - 2013

The Two Braggs Exhibition

Approximately 100 years ago in Germany Max Theodor Felix von Laue (1879-1960), Paul Karl Moritz Knipping (1883-1935) and Walter

Friedrich (1883–1968) showed that X-rays could be diffracted by crystals. Laue was subsequently awarded the Nobel Prize in Physics in 1914.

Following this discovery, the unique partnership, father and son, William Henry Bragg (1862-1942) and William Lawrence Bragg (1890-1971) in England, successfully showed how X-ray diffraction could lend itself to the solution of crystal structures, for which they shared the Nobel Prize in Physics in 1915.

To celebrate their achievements in this centenary year I am in the process of planning a major exhibition devoted to both of them as an adjunct to the ECM at the University of Warwick in the last week of August. The intention is to make it available not only to participants at the ECM, but also to the general public. The exhibition will show for the first time historic equipment (including the ionisation spectrometers designed by W.H. Bragg), their notebooks, photographs, honours (including Nobel certificates), and letters. Both Braggs were competent amateur artists and members of the Bragg family will be lending a number of their artworks for display.

Mike Glazer

The Structure of Stuff is Sweet

As part of the celebrations for the Centenary of Crystallography, the BCA, STFC and Diamond Light Source created an outreach stand for the Big Bang Fair in the eXcel Centre in London. This fair is held annually over four days, and attracts over 75,000 students and families to the venue to learn about science and engineering.

Our stand was called 'The Structure of Stuff is Sweet', and had many different interactive activities for all to enjoy.

The Structure of Stuff is Sweet exhibition, The Big Bang Fair, London

The fantastic replication of the Braggs' experiment using marbles by Mike Glazer proved to be particularly popular, as were the free marshmallow unit cells! Over 30 BCA members gave up their time and energy (including our very own President!) inspiring young and old alike to learn more about crystals and their intricate structures. The support from Neville Hollingworth at the STFC, Laura Holland at Diamond and particularly the tireless efforts of Ross Harrington (BCA Education Officer) made this whole event possible.

Mike Glazer working hard at The Structure of Stuff is Sweet exhibition

The fantastic volunteers and organisers were all vital to the success of this event, and the feedback from attendees was very positive. We have been approached to run further events, so keep your eyes peeled for more information in future BCA emails.

Clare Murray

You can catch 'The Structure of Stuff is Sweet' at the British Science Festival 9th-12th September.

International Year of Crystallography

As announced in the Autumn Newsletter, the UN has ratified that 2014 will be the International Year of Crystallography.

Efforts are being coordinated through the website, and members can take part by adding their events to the calendar and by contributing educational resources.

http://iycr2014.org/events

http://iycr2014.org/contribute/educational-materials

Display at Science Museum

Members may also be interested in a new display recently opened at the Science Museum, “Hidden Structures: 100 Years of X-ray Crystallography”.

This display celebrates the centenary of X-ray crystallography, a technique developed by father-and-son team William H. Bragg and W. Lawrence Bragg in 1913.

Opening in time for International Women's Day, “Hidden Structures” also discusses the complex role of women in molecular biology and displays key models by Kathleen Lonsdale and Dorothy Hodgkin.

Details for the display can be found at: http://www.sciencemuseum.org.uk/visitmuseum/galleries/crystallography.aspx

PCG-SCMP AGM

The 70th PCG-SCMP AMG will take place at the ECM28 conference at Warwick University on 29th August 2013 in the Ensemble room. Time will be confirmed once the session timetable for this date has been finalised.

The meeting agenda includes the following items:

- Apologies for absence
- Minutes of the 69th PCG-SCMP AGM held at Warwick, 18th April 2012
- Matters arising from minutes
- Chair’s report
- Treasurer’s report
- Elections to PCG-SCMP Committee
- Any other business

ACKNOWLEDGEMENT

I’d like to thank Clare Murray, Amber Thomson, Mike Glazer, Mark Senn and Ivana Evans for their contributions to the Newsletter.

Helen Maynard-Casely

PCG-SCMP COMMITTEE