

SIG6: Instruments and Experimental Techniques (IET SIG6)

Reported Period: 2010-2011

Report Date: 20-06-2011

Reported by: Jean-Louis Hodeau

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1. Introduction. (50 words max.)

The mission of SIG6 is to promote access and awareness of crystallographers to new instrumentations & methods and particularly those using synchrotron-radiation, FEL, neutrons and combined methods including crystallisation. Since this year, SIG6 has also suggested activities for diffraction physics and optics. SIG6 members have organised schools, conferences and symposia for ECM-Meetings, which are also outlined below.

2. SIG web site:

Since 2010, we have a SIG web site, the web master is Favre-Nicolin (F).

3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)

SIG6 Instrumentation and Experimental Techniques 88

4. Existence of a SIG mailing list: No

Address of the mailing list: we use of personal mail

Number of members in the SIG mailing list:

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate): 14

John R. Helliwell (UK), Ian Robinson (UK), René Guinebretière (F), Ake Kvick (S), Garcia Granda S. (SP), Kahn Richard (F), Saridakis Emmanuel (GR), Rodriguez-Carvajal Juan (F), Baumbach Tilo (D), Cernik Robert (UK), Vincent Favre-Nicolin (F), Heger Gernot (D), Naomi Chayen (UK), J-L Hodeau (F)

6. List of MS organized by the SIG at the last ECM

Title: Darmstadt ECM26 Microsymposia & Keynotes

IET-SIG6 gives a significant contribution to the Programme for the Darmstadt ECM26 in 2010. We proposed and organized or co-organised the following Keynotes and Microsymposia:

KEYNOTES

- **The European spallation source ESS**
Colin Carlile (Lund/SE)
Chair: Michael Steiner (Berlin/DE)
- **Resonant and coherent scattering on nanostructures**
Vincent Favre-Nicolin (Gif-sur-Yvette/FR)
Chair: Ulrich Pietsch (Siegen/DE)

MICROSYMPOSIA

- MS 38 : **Current trends in protein and small molecules crystallization and monitoring**
Chairs: Naomi Chayen (UK) E. Saridakis (GR)
- MS 39 : **Surfaces, interfaces and nanostructures**
Chairs : Gilles Renaud (F) X Torrelles (SP)
- MS 40 : **Micro- and sub-micro-diffraction**
Chairs : Henning Poulsen (DK) Jean Louis Hodeau (F)
- MS 41 : **Magnetism by neutrons and X-rays**
Chairs : T. Brueckel, (D) C. Vettier (Sweden)
- MS 42 : **Time-resolved X-ray diffraction and spectroscopy in biology and chemistry**
Chairs: Ronald Frahm, (D), M. Wulff (F)
- MS 47 : **Crystallography in Art and Archaeology**
Chairs : E. Dooryhee (USA) ; A. Thalal (Morocco)

Title: ECM27 Microsymposia & Keynotes

In Madrid, on August 2011, during the IUCr conference, we will meet together to prepare our suggestions to the Programme for the ECM27 in 2012.

7. Prizes sponsored/coordinated

Title: ECM26 Erwin Felix Lewy Bertaut Prize

In 2007, following suggestion of SIG member, the Erwin Felix Lewy Bertaut Prize was created by the European Crystallographic Association (ECA) and the European Neutron Scattering Association (ENSA) to young European scientists in recognition of notable experimental, theoretical or methodological contributions in the field of the investigation of matter using crystallographic or neutron-scattering methods. In 2010 at Darmstadt-ECM26, the third Prize (2000 euros) was attributed by Prof. *Michael Steiner*, President of ENSA and Prof. *Santiago Garcia Granda*, President of ECA to Dr. **Tom Fennell** for his work on "*Topological constraints in frustrated materials*".

At these occasions (both at the ECM25-Istanbul & ECM26-Darmstadt conferences) a poster dedicated on the memory of Erwin Felix Lewy Bertaut Prize was presented by SIG6 as a contribution by SIG6 to this important award.

Title: ECM26 Jacek Grochowski SIG6 poster Prize

Sponsors/Organizers: SIG6/University of Manchester and Daresbury SRS: for approx 1200 Euros (100 Euros per prize per ECM for purchase text in IUCr Crystallography Book Series or IUCr Int Tables Volume or personal subscription IUCr Journal e.g. *J of Applied Crystallogr* or *J of Synchrotron Radiation*). This prize for the best "Instrumentation & Experimental Techniques" poster is given in memory of Prof Jacek Grochowski who was greatly involved in SIG6 and in ECA. At ECM26 (SIG6 jury Jean-Louis Hodeau, Gernot Heger, Naomi Chayen, Juan Rodriguez-Carvajal & Bob Cernik), this Prize was attributed to **Vera Vasylyeva** from Inorganic Chemistry - Ruhr University - Germany, for his poster on "*Deuterium disturbs – Influence of deuterium on the aggregation of pyridine-N-oxides*".

The same SIG6 jury propose the MarResearch Prize to **Dr. Thomas White** from FEL - Hambourg - Germany, for his poster on "*Assembly of 3D intensities from femtosecond X-ray laser diffraction patterns*".

8. Past Activities other than Microsymposia at ECM

Title: HERCULES Course in Neutron and Synchrotron Radiation for Condensed Matter

21 February 2010 - 27 March 2010 Grenoble France

This five week course provides training for students, postdoctoral & senior scientists from European & non-European universities & laboratories, in the field of Neutron & Synchrotron Radiation for condensed matter studies (Biology, Physics, Chemistry, Materials Science, Geosciences, Industrial applications). It includes lectures, practicals & tutorials. It is an European school largely dedicated on methods & instrumentations using Synchrotron and Neutrons

Number of Participants : 79 students,

Chairs: J. Baruchel, D. Bellet, O. Isnard, J.L. Hodeau

and several SIG#6 lecturers Kahn R., Rodriguez-Carvajal J., Baumbach T., Heger G.

Title: FEBS Advanced Course 'Advanced methods in Protein crystallization' IV

26 June - 2 July 2010, Nove Hrad, Czech Republic

The conference was preceded by an associated crystallization workshop

N Chayen and other members of SIG6 are teaching

Title: Book published: "Macromolecular Crystallization and Crystal Perfection"

Oxford University Press 2010, by N.E. Chayen, J.R. Helliwell, and E.H. Snell

<http://ukcatalogue.oup.com/product/9780199213252.do>

Title: 3rd ILL Annual School on Advanced Neutron Diffraction Data Treatment using FullProf Suite

2-7 May, 2010, ILL, Grenoble France

These intensive, hands-on, schools are focus on the analysis of diffraction data with the FULLPROF SUITE and concern heterogeneous data coming from powders, single crystals, X-rays and time-of-flight neutron diffraction. FPSchool focus on the analysis of magnetic diffraction data: symmetry analysis, magnetic structure determination by simulated annealing, refinement of magnetic data as a function of temperature and refinement of single crystal data. It has taken place at the ILL and formed 29 participants.

Chair: J. Rodríguez-Carvajal; Co-chairs: M-H Lemée-Cailleau, G Cuello

SIG members involved in the organisation: J. Rodríguez-Carvajal

Title: HERCULES Hercules Specialised Course (HSC12) on " Synchrotron Radiation and Neutron for Extreme Conditions Studies"

27 September to 02 October 2010 Grenoble France

The purpose of this Hercules Specialised Course is to illustrate the basic principles of SR and neutron techniques used to explore matter at extreme conditions of pressure and temperature. The school will also provide cross-disciplinary examples covering fundamental physics, earth and planetary science, chemistry and material science. The lectures will cover both theoretical and experimental aspects for a non-expert audience. They will be complemented by tutorials and practicals at several ESRF and ILL beamlines and include an introduction to high pressure cell loading techniques

Chairs : Thomas Hansen (ILL) and Michael Krisch, Mohamed Mezouar, Sakura Pascarelli (ESRF)

Involvement of SIG6 member in the organisation: J-L. Hodeau

Title: ISDSB2010 3rd International Symposium on Diffraction Structural Biology

25 - 28 May 2010, University Paris-Sud, Orsay, near Paris, F

Organized on behalf of the University-Industry Cooperative Research Committee of Japan Society for the Promotion of Science (JSPS), for first time it was held outside of Japan

Chair: Prof. N. Sakabe ; Involvement of J. Helliwell (bursary applications to ECA and to IUCr)

Title: Crystallization workshop at International conference on the Crystallization of Biological Macromolecules.

9-12 September 2010, Dublin Ireland (<http://www.iccbm13>)

Drs L Govada and S Khurshid of N Chayen team teaching and N Chayen chair of the opening session of the conference.

Title: Crystallization workshop for European consortium MUZIC

21-22 November 2010, Vienna

Drs L Govada and S Khurshid of N Chayen team teaching

9. Future/Programmed Activities.

Workshop & schools on development of instrumentation even if such events are not officially ECA schools:

Title: HERCULES Course in Neutron and Synchrotron Radiation for Condensed Matter

28 february 2011 - 30 March 2011 Grenoble France

This five week course provides training for students, postdoctoral & senior scientists from European & non-European universities & laboratories, in the field of Neutron & Synchrotron Radiation for condensed matter studies (Biology, Physics, Chemistry, Materials Science, Geosciences, Industrial applications). It includes lectures, practicals & tutorials. It is an european school largely dedicated on methods & instrumentations using Synchrotron and Neutrons . Number of Participants : 82 students,

Chairs: J. Baruchel, D. Bellet, O. Isnard, D. Djurado

SIG members involved in the organizing committee (V. Favre-Nicolin, R. Kahn, J.L. Hodeau) and SIG#6 lecturers (Rodriguez-Carvajal J., Baumbach T).

Title: 4th ILL Annual School on Advanced Neutron Diffraction Data Treatment using FullProf Suite

- Basic session 24 - 28 January 2011, Grenoble
- Advanced session 30 Jan - 3 Feb 2011, Allevard, France

Precise crystallography has significantly contributed to the success and recent developments in materials science, solid state physics and chemistry. Among the available programs for diffraction data analysis, the FullProf Suite is one of the most widely used packages by the scientific community working in these fields. The aim of this annual school on the FullProf Suite (FPSchool) is to contribute directly to the training of the upcoming generation of scientists with intensive hands-on schools focused on the analysis of diffraction data using the FullProf Suite.

After three successful schools, we have decided to propose a new school organization. FPSchool-2011 will be split into two sessions in two places.

In order to favour intensive scientific exchanges, the number of students is limited to 30 for the basic session and 20 for the advanced one.

Chair: J. Rodríguez-Carvajal; Co-chairs: M-H Lemée-Cailleau, G Cuello

SIG member involved in the organisation: J. Rodríguez-Carvajal

Title: HERCULES Hercules Specialised Course (HSC13) “Industry” on “Neutrons and Synchrotron X-rays for Industrial Applications”,

2nd to 4th May 2011, Grenoble France

Successful innovation only starts with an invention or idea. Bringing it to fruition involves a deep understanding of many factors like growth and processing, scalability, manufacturing and machining, aging and shelf life. The unique properties of neutrons and synchrotron X-rays contribute to the innovation and product development chain, notably in the performance and properties of materials and the effects of processing. Non-destructive characterization is possible *in situ* and even *in operando*, without alteration of the sample, and even from samples buried deep in support structures.

This training course will give industrial scientists & technologists a privileged insight into the opportunities afforded by neutron & synchrotron X-ray beams to supply detailed information on the structure, microstructure and properties of materials. Public concerned : 1- Company Research Managers, 2-Industrial Scientists & Researchers, 3- Industrial Technologists, 4-Academic Scientists & Engineers collaborating with industrial partners.

Chairs : Jose Baruchel (ESRF), Andrew Harrison (ILL), Ed Mitchell (ESRF), Thilo Pirling (ILL), Jean-René Regnard (UJF & CEA Grenoble), Xavier Thibault (ILL)

Title: X-Rays and Neutrons in Energy-Related Materials Science

7-9 february 2011, ILL & ESRF, Grenoble, F

The development of new materials for energy relies to a large extent on a profound understanding of the multi-scale origins of their properties. Intense synchrotron X-ray and neutron beams, with their capacity to probe matter from the atomic to the macro scale, contribute significantly to this objective and are expected to play an even more important role in the future.

Chair: Prof. J. Baruchel ; Involvement of Juan Rodriguez-Carvajal

Title: British Crystallographic Association Spring Meeting 2011

11-14 April 2011, University of Keele

Involvement of John Helliwell as the BCA's 2011 Lonsdale Lecturer.

Title: REXS2011 Resonant Elastic X-ray Scattering for Condensed Matter

13- 17 June 2011, Aussois F (<http://rexs2011.grenoble.cnrs.fr>)

The first conference dedicated to Anomalous or Resonant X-ray Scattering took place in **Madrid in 1974** followed by a conference in **Malente in 1992**. The aim of these two conferences was to bring together scientists developing and using this technique specific to synchrotron radiation. The **2011 Resonant Elastic X-ray Scattering in Condensed Matter** conference/school (REXS2011) aims to bring together 120-130 scientists to cover the progress of the technique and trigger discussions about future applications, in particular at new light sources. Selected keynote lectures will ensure the didactic content, while more specific invited talks will complete the scientific view of a field and/or present new possibilities.

Topics covered are : 1- Fundamentals of elastic resonant scattering, 2- Electronic correlations, 3- Magnetism, 4- Nanostructures, 5- Soft condensed matter, polymers and glasses, 6- Materials science and chemistry and 7- Instrumentation

Techniques addressed cover : diffraction, reflectivity, small, wide angle, grazing incidence x-ray scattering, diffraction anomalous fine structure, magnetic scattering, coherent scattering

Chair: J-P Simon (CNRS) C. Mazzoli (ESRF) T. Schulli (ESRF), with a strong involvement of SIG6 members

J.L. Hodeau and V. Favre-Nicolin.

Title: European Lab Automation, including Advances in Protein Crystallography

30 Jun-1 Jul 2011 , Hamburg, Germany (<http://www.selectbiosciences.com/conferences/APC2011/>)

The congress will consist of ten distinct tracks (see right), each addressing a specific application area, but with an underlying theme of automating the technique, equipment or associated informatics. The **Advances in Protein Crystallography present four main topics** : 1- Protein Chemistry and Crystallization, 2- New Laboratory Instrumentation; 3- Crystallographic Computing; 4- Fragment Based Lead Discovery with a strong involvement of SIG6 member Naomi Chayen

Title: European Lab Automation Crystallization Training Course

30 Jun-1 Jul 2011 , Hamburg, Germany(http://www.selectbiosciences.com/conferences/ELA2011/Training_Courses.aspx)

Drs L Govada and S Khurshid of N Chayen team teaching

Title: Mieres 2011: Crystallographic Computing School

16-22 Aug 2011, Oviedo, Spain

(<http://www.iucr.org/resources/commissions/crystallographic-computing/schools/mieres2011>)

This school is open to all crystallographic community (including macro- and small-molecule crystallography, powder diffraction, and small-angle scattering). It will put a strong weight on fostering one-on-one interactions. Accordingly, there will be only 16 lectures of 45 minutes each plus 6 student lectures of ~20 minutes, (14 hours total) but more than 24 hours of tutorials in small groups.

School organisers : Prof Santiago García Granda, Dr Harry Powell, et al. ; with a strong involvement of SIG6 member Prof Santiago García Granda team organization, V. Favre-Nicolin team teaching

Title: JCNS 2011 "Trends & Perspectives in Neutron Instrumentation: From Continuous to Spallation Sources"

4-7 October 2011, Tutzing, Germany (http://www.jcns.info/Workshop_2011/)

With new spallation sources taken into operation in the US and Japan, as well as with the decision to build the long-pulse spallation source in Europe, the centre of gravity in developments of neutron instrumentation is shifted towards the spallation source one. The aim of the workshop is to discuss this transition from the point of view of the most effective use of the knowledge accumulated during the design/construction of modern instruments at continuous sources as well as from the use of first instruments at spallation sources.

with a strong involvement of SIG6 member G. Heger

Title: 9ème Colloque Rayons X et Matière

28 november - 01 december 2011, Tours F

The objectives of this meeting were to bring together the community of material & metallurgy sciences to use new X-ray, neutron and SR method by the F community, a special focus will be given for chemistry applications.

For the International year of crystallography, a large public exhibition " le Cristal in bijou pour la Chimie" will be created

Chair: Prof. R. Guinebretiere, P. Goudeau, and strong involvement of J.L. Hodeau and R. Guinebretiere.

10. Other matters. (50 words max.)

One of the missions of SIG6 is also to promote access and awareness of crystallographers to new sources and SIG6 members have encouraged scientists to be involved on new XFEL sources. SIG6 strongly supports the detector developments, particularly on pixel detectors and we will propose a dedicated microsposium at ECM27.

11. Brief annual activity report (100 words max.)

SIG6 members usually communicate via emails, during some large facility user meetings and during ECM meeting. In 2010, SIG6 was involved in the organization of two keynotes and several microsypomia at the ECM-26 Darmstadt. SIG6 members have organized several schools and workshops like: School on Advanced Neutron Diffraction Data Treatment, HERCULES Course in Neutron and Synchrotron Radiation for Condensed Matter and several HERCULES Specialised Courses. SIG6 supports requests of financial supports for the International School/Conference on Resonant Elastic X-Ray Scattering in Condensed Matter in Aussois –France and, recently, the Erice – Italy conference on "Present and Future Methods in Biomolecular Crystallography".

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

Secretary : Heger Gernot (D) "Heger Gernot" <heger@xtal.rwth-aachen.de>

Vice-Chair : Naomi Chayen (UK), "Naomi Chayen" <n.chayen@imperial.ac.uk>

Chair : J-L Hodeau (F) "Hodeau jean Louis" <hodeau@grenoble.cnrs.fr>

As the present chair had served several years, at IUCr Madrid meeting, SIG6 chair will change.

Supplementary Materials. None