

SIG6: Instruments and Experimental Techniques (IET SIG6)

Reported Period: 2009-2010

Report Date: 30-05-2010

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 *Instruments and Experimental Techniques*. This concerns instrumentations & methods and particularly those who use synchrotron-radiation, FEL, neutrons and combined methods. Our main activities in 2009-10 have been to organise schools, conferences and symposia for the ECM-Meetings.

2. SIG web site:

SIG6 Not yet; in 2010, we will implant a SI6 web site (Favre-Nicolin (F) is our new web master)

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 63

4. Existence of a SIG mailing list: No

Address of the mailing list: 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): 11

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

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

Title: ECM25 Microsymposia & Keynotes

IET-SIG6 organized or co-organised with other SIG the following Microsymposia.

KEYNOTES

- Complementarity of Magnetic Neutron and X-ray Scattering

Lecturer: Thomas Brückel ; Chair: Dincer Ulku

MICROSYMPOSIA (86 contributions)

FA5-MS3 Remote Experimentation , Telepresence and Automation

Chair: Simon Coles ; Co-chair : Roberto Pugliese (5 orals & 4 posters)

Alun Ashton A Facility Wide Solution to Remote Experimentation and Automation

Peter Turner Remote Access: The Virtual Scientific Instrument and The Web

Santosh Panjekar Auto-Rickshaw: A Tool for Online Validation of X-Ray Diffraction Experiment

Gordon Leonard Automation and Remote Access on the ESRFs Macromolecular Crystallography Beamlines

Miroslaw Gilski Remote Synchrotron Data Collection and Structure Determination Pipeline

FA2-MS8 Coherent X-Ray diffraction and Imaging of materials

Chair: Sylvain Ravy ; Co-chair: Bob Cernik (5 orals & 4 posters)

Virginie Chamard Strain Imaging at the Nanoscale with Coherent X-ray Diffraction

Simon Jacques Monochrome and Colour X-ray Diffraction Imaging

Vincent Jacques Towards Imaging of Topological Defects by Coherent X-ray Diffraction

Moreton Moore Imaging Diamonds with X-rays

Felisa Berenguer Coherent Xray Diff. Imaging of Antiphase Domains & Bio Tissues with Ptychography

FA2-MS6 Surfaces and Interfaces

Chair: Wolfgang Donner ; Co-chair: Mustafa Oksuzoglu (5 orals & 13 posters)

Andreas Stierle Shape Reconstruction of Nanoparticles under Reaction Conditions

John N. Chapman The Influence of Interfaces on the Properties of Magnetic Nanoelements and Wires

Amall Ahmed Ramanathan Structure & Magnetism of Fe/Mo(001) Surface: A Pseudopotential Calculation

Matej Jergel GISAXS-based Optimization of La/B4C Multilayer Mirrors for Soft Xray FEL

Mehmet Erbudak Structure of the Surface Oxides Grown on the Icosahedral Al-Pd-Mn Quasicrystal

FA5-MS 4 Synchrotron Radiation based Crystallography & Spectroscopy in Middle East

Chair : Samar Hasnain ; Co-chair : Engin Ozdas (5 orals & 2 posters)

Messaoud Harfouch XAFS Study of Actinides in Minerals Analogues of Ceramics for Nuclear Waste

Moazut Rahman Efforts for Structural Biology of Membrane Proteins in a SESAME member country

Filiz Yesilirmak Use of Modified Metallothioneins for Biosensor Application

- Mervat Hassan** Aspects of Crystallinity of High Grad Quartz Ores Using X-Ray Diffraction and Infrared Spectroscopy Diagnostic their chemical reactivity
- Mehmet Aslantas** Protein Crystallography: Counter Diffusion Crystallization Method and Its Potential for Room-Temperature Data Collection
- FA2-MS 9 Combination of Synchrotron and Neutrons in Magnetic Materials
Chair: Markus Braden ; Co-chair: Yalcin Elerman (5 orals & 5 posters)
- Christian Schuesler-Langeheine** Resonant Soft X-ray Diff. as a Probe for Complex Magnetic Structures
- Mehmet Acet** The Nature of Magnetic Coupling in the Martensitic and Austenitic Structures in Magnetic Shape-Memory Alloys Studied by Neutron Polarization Analysis
- Andrew Sazonov** Orbital Contribution to the Magnetic Moment in Co₂SiO₄
- M. Bakr** Structural, Magnetic and Electric Properties of GaFe_{1-x}Mn_xO₃
- Manfred Reehuisa** Neutron Diffraction Study of DyVO₃ and HoVO₃
- FA2-MS 3 Crystallography in Art and Archaeology
Chair : Eric Dorryhee ; Co-chair: Petr Bezduka (5 orals & 6 posters)
- Dario P. Benedetti** X-ray Techniques Applied to Art Authentication and Conservation
- Manfred Schreiner** The Hoard of Becin the Silver Content of the Akce Coins and the Monetary History of the Ottoman Empire
- Lindsay Sawyer** Crystallography and Industrial Design: Past, Present & Future
- David Hradil** Mineralogical and art-historic traits in the investigation of anonymous paintings
- Annegret Haake** The Javanese Colleagues of Karagöz and Their Dress
- FA3-MS 1 Coherent X-ray Diffraction and Imaging in Biology
Chair : Tim Salditt; Co-chair : Edgar Weckert (5 orals & 3 posters)
- Duane Ne-Te Loh** A reconstruction algorithm for single-particle diffraction Imaging experiments
- Yoshinori Nishino** Visualization of cells and cell organelles using coherent x-ray Diffraction
- John Miao** Coherent X-ray diffraction imaging of biological specimens
- Enju Lima** Cryogenic x-ray diffraction microscopy with hard x-rays for biological samples
- Axel Rosenhahn** Lensless imaging of biological samples with soft x-rays
- Klaus Giewekemeyer** Highly sensitive quantitative biological imaging by scanning x-ray diff. microscopy
- FA3-MS 4 Time Dependent and In-situ Neutryshyn
Chair: Poul Norby ; Co-chair: Anatoliy Senyshyn (5 orals & 9 posters)
- Paul Barnes** Observing Functional Materials in Operation Using Time/space-resolved Diffraction
- Klaudia Hradil** Kinetics of Solid State Reactions/Transitions Investigated by RealTime Neutron Spectroscopy
- John Richard Helliwell** Time-resolved binding of K₂PtBr₆ to lysozyme by protein powder and single crystal
- Oleg Schmidt** X-ray Diffraction Study of Piezoelectric Crystal Response on the Nanosecond Time Scale
- Lea Nichtova** In-Situ Study of Time and Thickness Dependence of Crystallization of Amorphous TiO₂ Thin Films and Powders

Title: ECM26 Microsymposia & Keynotes

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

KEYNOTES

- **Resonant and coherent scattering on nanostructures**
by Vincent Favre-Nicolin (FR)
- **The European spallation source ESS**
by Colin Carlile (SE)

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. Dorryhee (USA) ; A. Thalal (Morocco)

7. Prizes sponsored/coordinated

Title: ECM25 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 2009, the second Prize (2000 euros) was attributed at the ECM25-Istanbul conference to Dr. **Lukáš Palatinus**. At this occasion a poster dedicated on the memory of Erwin Felix Lewy Bertaut Prize was made by SIG6. The third prize will be given in 2010 at Darmstadt-ECM26

Title: ECM25 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 ECM25 (jury Naomi Chayen, Emmanuel Esaridak, Bob Cernik), this Prize was attributed to **Ricardo Miguel Ferraz Leal**, from the *ESRF-Grenoble-F and the EPSAM Keele University UK*, for "Absorption Correction and Optimal Planning of Data Collection Based on a 3D Sample Model"

8. Past Activities other than Microsymposia at ECM

Title : 13th JCNS Laboratory Course – Neutron Scattering

7-18 September 2009 Jülich/Garching – Germany

These courses were organized by Forschungszentrum Jülich with RWTH Aachen & WWU Münster. They consist of lectures & experimental section. The lectures gave an introduction to neutron sources, into scattering theory and instrumentation. Furthermore, selected topics of condensed matter research were presented. The course gave a realistic insight into the experimental technique neutron scattering and its scientific power.

Chairs : T. Brückel, G. Heger, D. Richter, R. Zorn

Title: HERCULES Course in Neutron and Synchrotron Radiation for Condensed Matter www.aaa.com

1 March 2009 - 4 April 2009 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 each year: 83 students,

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

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

Title: 2nd ILL Annual School on Advanced Neutron Diffraction Data Treatment using FullProf Suite

26-30 January 2009 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-2009 will 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 Institut Laue-Langevin and formed 25 participants.

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

Title: 20th International Congress on X-Ray Optics and Microanalysis

September 15-17, 2009, Karlsruhe, Germany

The ICXOM series is dedicated to the fields of X-ray optics and micro (nano) analysis by means of X-ray beams (with an emphasis in 2009 on synchrotron sources), electrons or other energetic particles. It is meant as a platform for discussion and exchange for users and experts involved in these fields. At the **ICXOM20** meeting in Karlsruhe, it were given presentations, demonstrating recent progress in fundamental and applied research in X-ray optics and micro & nano analyses, methodological and instrumental developments.

ICXOM20 was organized by various institutes of FZK (INE, ISS and IMT) in collaboration with ITU and University of Karlsruhe by Tilo Baumbach ANKA

Title: Second International School on Biological Crystallization

18 May 2009-22 May 2009 Granada Spain

This International School has focused on the fundamentals of crystallisation from solutions and its applications to the field of the crystallisation of biological materials. The School has provided five days of lectures and practical demonstrations related to the crystallisation of biological macromolecules, biominerals & biomimetic materials, with one day devoted to case studies on the crystallisation of membrane proteins and large macromolecular complexes.

Chair: J.M. Garcia-Ruiz

Title: Sixth Interdisciplinary Transport Phenomena Conference

4-9 October 2009, Tuscany, Italy

This was the sixth Conference in covering Interdisciplinary Transport Phenomena organized in cooperation with the Engineering Conferences International. The conference has covered topics in Transport Phenomena in relation Fluid, Thermal, Biological, Materials, and Space Sciences.

Involvement & Keynote: Prof. N Chayen

Title: 8^{ème} Colloque Rayons X et Matière

8 - 11 december 2009, Orsay 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.

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

Title: HERCULES Hercules Specialised Course (HSC10) on " Synchrotron radiation techniques contribution to nanoscience" www.aaa.com

18 to 22 May 2009 Grenoble France

Using synchrotron sources for nanosciences is already well developed and keeps improving since these sources and their instrumentation are constantly progressing and are more adapted to a large range of studies conducted on semiconductors, magnetism and biomedicine. HSC10 has covered all these different aspects.

Chairs : J. Baruchel, M. Burghammer, T.H. Metzger, S. Pascarelli

Title: HERCULES Hercules Specialised Course (HSC11) on "Application of Neutron & Synchrotron Radiation to Magnetism" www.aaa.com

16 to 20 November 2009 Grenoble France

Since the 1940s, neutron scattering has been an essential tool for the investigation of magnetic structures & dynamics. More recently, the intensity and flexibility of synchrotron radiation has been exploited for application to research in magnetism. Developments in instrumentation & techniques mean that the two forms of radiation can be used to give complementary detailed information never seen before. HSC11 has covered these different aspects. Chairs : N. Brookes (ESRF), A. Wildes (ILL)

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 www.aaa.com

21 february 2010 - 27 April 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 Hradý, 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

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 be 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 in a representative range of scientific areas, 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)

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)

10. Other matters. (50 words max.)

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

Commission members usually communicate via emails, informally during some large facility user meetings and formally during ECM meeting. In 2009, SIG6 was involved in the organization of eight microsymbiosia at the ECM-25 Istanbul-2009 with 86 contributions. For the future ECM26-Darmstadt-2010, it was also highly involved. SIG6 members have organized several schools and workshops like: Annual School on Advanced Neutron Diffraction Data Treatment using the FullProf Suite, FEBS Advanced Course 'Advanced methods in Protein crystallization', 13th JCNS Laboratory Course in Germany, HERCULES Course in Neutron and Synchrotron Radiation for Condensed Matter and several HERCULES Hercules Specialised Course (HSC).

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>

Supplementary Materials. none