ESRF Users' Meeting 2010: reports from parallel sessions

General remarks:

A session of the plenary part of the Users' meeting was dedicated to feedback from the parallel sessions and open discussion with management. Here some points issuing from the discussions of the parallel session and of concern for all, or most, of the Users groups.

- Beamtime Review Committees should give some indication about why a proposal was refused. Users need to know where they can improve their proposal, or if their proposal is simply too irrelevant to be accepted. If a proposal is sound, but refused because of lack of available beamtime, the proposer should be informed about the problem and encouraged to resubmit the proposal.
- The ESRF network should be improved and faster data transfer assured
- Users need to be informed about relevant technical improvements, new equipments and techniques present at the ESRF; the new Instrumentation Services and Development division could likely report on this during the annual Users' Meeting
- Users would like to benefit from ESRF software development at home. Data analysis software might occasionally be downloadable through NICE, but the procedure how to access those tools is not at all trivial
- The User community sustains entirely all collaborations between facilities, which, in the every end, will push forward the technology enabling the very best science produced by Users
- The Users' community is very favourable of a European-wide common User Interface (SMIS), which should facilitate the access to various, sometimes complementary, facilities
- The Surfaces & Interfaces group desires to continue to exist, even if only on a informal basis, ex. Parallel Session at the Users' meeting
- The quality of the canteen at evenings and during week-ends should be improved. The guesthouse, especially Building A, should be refurbished, especially for what concerns sanitary installations.
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STRUCTURE OF MATERIALS

Organisers and Chairs: Chiara Maurizio (Users Organization & Italian CRG), Andy Fitch (ESRF Group Leader)

The Structure of Materials Parallel session was attended by more than 30 people.
A first set of brief talks was dedicated to present news from the ESRF beamlines ID31 (A. Fitch), ID15 (V. Honkimäki), ID09B (M. Wulff), ID11 (J. Wright). This part was followed by four scientific talks, given by young and skill scientists that overviewed different topics in the wide field of the Structure of Materials. Simon Kimber (Helmholtz Zentrum, Berlin, Germany) spoke about the orbital and change ordering of ruthenates as observed by high resolution x-ray diffraction. The following two talks were about proton-conducting oxide and membranes for fuel-cells (Francesco Giannici from Palermo University and Barbara Paci from CNR-Roma, Italy); the last

talk was given by Maciej Lorenc (Rennes University, France) on the dynamics of bistable spin-crossover molecules at solid state. Each talk was followed by questions and comments. The last part of the parallel session was a sort of round table to discuss needs of the ESRF users and/or ways to improve the scientific users' life at the ESRF. The main points raised were about i) network improvements, including a faster data transfer; ii) the need to be informed about relevant technical improvements, new equipments and techniques present at the ESRF; the new Instrumentation Services and Development division could likely report on this during the annual Users' Meeting.

ELECTRONIC STRUCTURE & MAGNETISM

Organisers and Chairs: Paolo Ghigna (User Organisation & University of Pavia, Italy), Carmela Aruta (User Organisation & CNR-INFM, Napoli, Italy), Nick Brookes (ESRF Group Leader)

The parallel session on Electronic Structure & Magnetism was attended by about 40-50 people.
The aim of the session was to give recent highlights presented by users. For this purpose, four speakers were invited from different fields of research using different techniques and they showed results obtained at the ESRF on several beamlines belonging to the ESM area.

The first invited talk was presented by Marco Salluzzo (CNR-INFM Coherentia, Napoli, Italy). The title was "Orbital reconstruction and 2D electron gas at the interface between $LaAlO_3$ and $SrTiO_3$". It was shown that the generation of a conducting electron gas is related to an orbital reconstruction occurring at the $LaAlO_3/SrTiO_3$ interface. The results were obtained by using x-ray absorption spectroscopy measurements with different linear polarizations performed at ID08.

The second invited talk was given by Federica Fabrizi (ESRF, Grenoble, France and University College, London, UK). The title was "Circularly Polarized X-ray Magnetic Scattering as a probe of Multiferroic Materials". The speaker showed measurements performed at ID20 by combining magnetic non-resonant diffraction by circularly polarized X-rays with the full linear polarimetry of the scattered beam, both on $TbMnO_3$ and $Ni_3V_2O_8$. It was shown that the complex magnetic structure of such multiferroic samples was further refined.

The third invited talk was given by Matthias Bauer (Universität Stuttgart, Germany). The title was "Homogeneous catalysis and X-ray spectroscopy: Methods, timescales and perspectives". Several spectroscopic techniques such as EXAFS, XANES, Raman and UV-Vis studies were shown to study homogeneous Iron- and Cerium-based catalytic reactions. Dispersive XAFS measurements at ID24 on copper catalyzed reaction and RIXS and XES measurements were also showed.

The last invited talk was given by Andreas Ney (Universität Duisburg-Essen, Germany). The title was "Probing the local structural and magnetic properties of dilute magnetic semiconductors using hard X-ray absorption spectroscopy". It was

shown the study of the lattice sites occupation and the magnetic properties in Gd:GaN and Co:ZnO dilute magnetic semiconductors by x-ray linear and magnetic circular dichroism, performed at ID12 beamline.

Pertinent questions and interesting discussions followed all the invited talks.

The final discussion focused on the upgrade program was introduced by a talk of Nick Brookes, the head of the ESM group, who informed about the new aspects of the ESRF upgrade program involving the beamlines of the ESM area.

STRUCTURAL BIOLOGY

Organisers and Chairs: Gerlind Sulzenbacher (User Organisation & CNRS-Univ. Marseille), Sean McSweeney (ESRF Group Leader)

The Structural Biology (SB) parallel session was integrated with the school entitled "Getting the most from the ESRF MX beam lines" and held in the PSB Seminar Room of the Carl-Ivar Brändén Building, with an attendance of about 60 people. The aim of the session was to give the Users an overview of present, short term and long-term developments and research opportunities at ESRF, to focus on the principle challenges of Structural Biology in the future and how these challenges can be addressed by Instrument and Methodology developments, and finally to give Users the opportunity to present their work.
The session started with a talk by Mathew Bowler, beamline scientist on ID14-2, on how to get the best data from a sample by using on-line dehydration and diffraction cartography. The session carried on with a presentation of the Upgrade Programme for the Structural Biology beam lines at the ESRF by Christoph Müller-Dieckmann, beamline scientist on ID29. Adam Round, beamline scientist on ID14-3 gave an overview of the new Bio-SAXS beamline. The methods and instrumentation part ended with a talk by Trevor Forsyth, ILL, on the use of Neutrons in modern Structural Biology.
The talk by users were as follows: Carlo Petosa, IBS, Grenoble: "Structure of a BET-family bromodomain bound to a diacetylated histone tail"; Nathalie Colloc'h, CI-NAPS, Caen: "Crystallographic studies under inert gas pressure at room temperature on beamlines BM14 and BM16, and pressure-response analysis of inert gas binding mode"; Clement Blanchet, EMBL-Hamburg: "CryoSAXS Sample environment"; Annabelle Varrot, CERMAV, Grenoble: "Characterization of a superlectin from Burkholderia cenocepacia". The parallel session ended with a very joyful Poster-clip session, where students participating at the school had three minutes each to present their work.
Just before talk by Users about forty minutes were dedicated to discussion. The major points arising form the discussion can be resumed as follows:

- Users are generally very happy on how the Structural Biology beamlines are run
- Users perceive very positively the Upgrade Programme for the Structural Biology beam lines
- Users realize that the Upgrade represents a huge workload and worry that if adequate staffing is not assured by the ESRF, they might not benefit from the

same assistance they were used to in the past, and that consequently their scientific throughput might be compromised
- The main problem for Users of the Structural Biology community is to produce well diffracting samples. In order to tackle the most challenging problems by extracting very weak signals it is mandatory that the Structural Biology beamlines should be equipped with the best detectors available
- In the view of massif data throughput in the future Users feel that the rate of data transmission should be enhanced
- Safety rules are sometimes too strict or meaningless (ex. a sample containing pico-molar amounts of lead (!!!) needs to be declared much in advance as a sample containing hazardous ligands
- And last not least: whereas quality of the canteen food is good standard at lunchtime, the quality and availability of food is sometimes appalling in the evenings or during the week-ends

SURFACES & INTERFACES SCIENCE

Organisers and Chairs: Christian Kumpf (User Organisation & Research Center Jülich, Germany), Jörg Zegenhagen (Beamline Responsible ID23)

This year the parallel session on "Surfaces and Interfaces Science" was attended by up to 70 people. Compared to the years before the session was extended, and was continued after the afternoon coffee break. This format allowed additional reports from the beamlines (the bending magnet beamlines were included for the first time) and longer talks given by invited users.

After a short welcome the session started with a contribution by Tobias Schülli, the new responsible scientist at ID01. He reported on coherent diffraction experiments on InAs, 3D Bragg holography and on present and future developments at ID 01. Afterwards Gilles Renaud (BM32) introduced a Fourier-analysis method for reflectivity measurements yielding the density profile of multilayer systems. In the following short contribution Roberto Felici described present and future developments at ID03.

Andreas Biermanns from Siegen University (Germany) then gave the first user's contribution. In a very interesting talk he reported on "focused beam dark field imaging" experiments performed on GaAs nano-rods grown on a GaAs substrate. Rods and substrate show different lattice spacing, even though the lattice mismatch should be vanishing. He used coherently scattered radiation from individual rods which were selected by Fresnel zone-plate focusing of the beam. The second user's talk was given by Pascal Andreazza (CNRS & Université d'Orléans). His topic was bimetallic CoPt and FePt nanoparticles which were investigated by WAXS and SAXS at BM32 and ID01. The phase diagrams as well as order-disorder transitions in the particles were discussed.

After the coffee break two more beamline-contributions followed: Juan Rubio-Zuazo reported on BM25B and its specific equipment for surface science experiments and on

new setups at the beamline, mainly regarding the z-axis diffractometer. Afterwards Jörg Zegenhagen gave an overview on the present situation at ID32. He concentrated on the new HAXPES and XSW machine and the possibilities which are enabled by the new high-energy analyzer. News from the diffractometer end station was also part of the presentation.

The final contribution was given by Jochim Stettner from Kiel university, Germany. He reported on time-resolved XRD studies on the Au(111) surface and its modifications under homoepitaxial electrodeposition. A time resolution of 5 msec was reached in the experiments and enabled recording growth oscillations at a dissolution rate of up to 11 layers/sec.

Finally it should also be mentioned that, beside the scientific debate, the surface/interface science community also discussed the recent changes in the structure of the internal ESRF groups. So far the subjects of the parallel sessions at the users meeting mirrored to the ESRF group structure. However, based on the size of the community and the long-time experience with the format of the parallel sessions, the community clearly expressed the necessity of preserving the actual format, i.e. the parallel session shall be kept alive in future, even though no corresponding ESRF group exists any more. This request was forwarded to the ESRF management in the feedback and discussion session on the second day of the users meeting. Since the management fully agreed with the communities opinion, the user's organization will continue with the successful series of parallel session on surface- and interface science at the ESRF user's meetings in future.

X-RAY IMAGING

Organisers and Chairs: Eric Maire (User Organisation & INSA, Lyon, France), José Baruchel (ESRF ESRF Group Leader)

The parallel session of the imaging group of the 2010 ESRF User's meeting gathered 30 to 40 attendees.

The scientific program included information from the beam lines staff, represented by Jose Baruchel, who gave an overview of the situation of the imaging beam lines in the frame of the upgrade program. The scientific program was grounded on different highlights of the studies carried out by users and ESRF staff during the current year. This program, lively and nicely illustrated during three talks, covered paleontology, fast experiments and medical imaging. The three talks were of very high quality, and anyone could judge the next day, listening to Phil Wither's talk in the plenary session who gave another overview of our research field, that many different academic and industrial applications are concerned. The session ended with a general discussion of the concerns of the users. These concerns were reported the next day in the closing plenary dicussion. They include data transfert and fast data reconstruction, typical problems of the imaging group. The imaging users community also agreed to give a

general support to the paleontology initiative, as an outstanding illustration of how a discipline can be revolutionized by 3D imaging, possible at the synchrotron sources.

SOFT MATTER STRUCTURES

Organisers and Chairs: Stephan Roth (User Organisation & HASYLAB Hamburg, Germany), Olivier Diat (User Organisation & ICSM, Bagnols s/Céze, France), Theyencheri Narayanan (ESRF Group Leader)

14:00 - 14:20 Introduction & Presentation of the Upgrade
Teyencheri Narayanan, ESRF, Grenoble, France

14:20 - 14:50 Presentation of the Upgrade

Anders Madsen & Oleg Konovalov, ESRF, Grenoble, France

14:50 - 15:00 Discussion

15:00 - 15:30 SAXS from protein solutions on ID02 - experiences with large multidomain proteins and their ligand interactions
Steve Perkins, University College London, UK

15:30 - 16:00 Slow relaxation in colloidal mesophases
Doru Constantin, Lab. de Physique des Solides, Université Paris Sud, Orsay, France

16:00-16:30 COFFEE BREAK

16:30 - 17:00 Mesostructured polymer-surfactant film formation at the air-solution interface
Karen J. Edler, University of Bath, UK

17:00 - 17:30 A microdiffraction study on the confinement effects in one-dimensional polymer arrays
MariCruz Garcia-Gutierrez, Instituto de Estructura de la Materia, CSIC, Madrid, Spain

17:30 - 18:00 Discussion

DYNAMICS & EXTREME CONDITIONS

No parallel session has been organized for this field. Interested Users have been invited to join the workshop on "Science at High Pressure: Initiative for the creation of a ILL/ESRF Partnership for Extreme Conditions Science" ("PECS workshop")