

ESRF Users' Meeting 2008: reports from parallel sessions

MACROMOLECULAR CRYSTALLOGRAPHY SESSION

Organisers and Chairs: Gerlind Sulzenbacher (User Organisation and Univ. Marseille), Sean McSweeney (ESRF)

The Macromolecular Crystallography (MX) parallel session was integrated within a workshop on "Structural and Molecular Biology of Host-Pathogen Interactions", jointly organised by ESRF, IBS, EMBL and UVHCI and held in the ESRF Auditorium. Approximately 50 people attended the parallel session. The parallel session had two objectives – firstly, to give the Users an overview of present, short term and long term developments and research opportunities at ESRF in the field of Macromolecular Crystallography; secondly, to inform the Users about the ESRF Upgrade and the outcome of the discussions held during the Upgrade meeting on October 23-24 2007.

The session started by a talk given by Johan Turkenburg, YSBL, University of York, about Remote Data Collection. Johan has tested thoroughly this mode of access and he was able to convince the audience of the benefits of remote access for standard experiments. The session carried on with two presentations by Petra Pernot, ESRF: the first about Biological SAXS and the second about Biological Coherent Diffraction Imaging – recent status in the ESRF and around the world. Finally, Sean McSweeney gave an overview of the Upgrade Programme and the session was concluded by a lively discussion. The major points arising from the discussion can be resumed as follows.

- Current MX operations represent 45 % of the ESRF users visits and gives rise to a substantial number of publications in high impact factor journals. Given this large percentage and the increased scientific throughput obtained over the last few years Macromolecular Crystallography should be considered as a main line of research activity at the ESRF.
- In the future the community will need an increased amount of beam time for extensive screening of a large number of samples in order to identify the samples suitable to determine the 3-D structure of particularly challenging targets.
- This need is well addressed by the "MASSIF" CRD, a multiple end-station beam line, which will allow extensive screening and subsequent sample dispatching.
- Given that automation of MX beam lines is well advanced and will even more improve in the future, the through-put will be huge and hence sufficient floor space is required in order to manage the enormous amount in-coming and out-going dewars used for sample shipping. Only by locating "MASSIF" at a long beam line the above requirement can be fulfilled.
- The idea of the creation of an MX village has been well received. This village, organized around "MASSIF" and grouping tunable beam lines with variably focused beams and a biological SAXS beam line could address the future needs of an integrative approach to structural biology.

SURFACE AND INTERFACE SCIENCE PARALLEL SESSION

Organisers and Chairs: Chris Lucas (User Organisation and University of Liverpool), Christian Kumpf (University of Würzburg, Germany & Users Organisation), Jörg Zegenhagen (ESRF)

The parallel session on Surfaces and Interfaces science was attended by approximately 50-60 people. Three (ESRF-) internal and three external contributions were scheduled. Due to lively discussions during the interesting session the timetable was overrun by almost 20 min.

The program started with rather technical contributions by the ESRF staff. Jörg Zegenhagen gave an overview over the “News from the SIS Group”, most prominent a new monochromator at ID01, a new catalysis chamber at ID3 and the new electrochemistry lab facility. Afterwards Ana Diaz (ID1) and Didier Wermeille (ID3) concretized the present situation at the beamlines and reported on research opportunities with coherent radiation, submicron focusing and surface X-ray diffraction including some research highlights in their fields.

In the second part of the session three scientific contributions from invited speakers were given: Vincent Favre Nicolin (CEA, Grenoble, France) showed very nice results using grazing incidence and coherent X-ray diffraction on semiconductor nanowires. The growth, crystallinity and surface-faceting of the nanowires can be investigated in detail using these techniques. The impact of the results was also highlighted by the plenary speaker of the morning session, Ian Robinson (London Centre for Nanotechnology). Afterwards Maddalena Pedio (TASC-INFN, Trieste, Italy) reported the adsorption of C₆₀ molecules on differently oriented Au and Ag surfaces. X-ray experiments revealed the bonding geometry of C₆₀ with the surfaces and allowed to draw conclusions on the interaction mechanism. An ordered nanostructuring of the metal surfaces (induced by the adsorbed molecules) was also found. In the final contribution Jeroen van Bokhoven (ETH Zurich, Switzerland) showed how X-ray standing waves can be utilized to identify active sites in zeolites, an important question for the understanding of the efficiency of these materials in applications. In a proof of principle-experiment the aluminum occupation of T-sites was measured for a scolcrite sample.

MATERIALS SCIENCE PARALLEL SESSION

Organisers and Chairs: Alain Lodini (User Organisation and Univ. Reims), Chiara Maurizio (ESRF, CRG & Users Organisation), Andy Fitch (ESRF)

The afternoon for the materials science parallel discussion group was densely packed with contributions. After the 2-minutes contributions from the scientists in charge of the beamlines composing the materials science group (ID09A, ID09B, ID11, ID15, ID27, ID31), seven talks were given by researchers working in different European universities and research centers. The discussion was particularly fruitful thanks both to the variety of the topics addressed in the talks and to the quality of the reported results, partly also presented by very young and promising researchers.

Several topics, as the investigation of stress and strain in materials, the structure of optical waveguides, laser-excited protein molecules, Earth's deep interior and superconductivity, have largely demonstrated to take all advantage from synchrotron radiation experiments, based either on diffraction and time resolved scattering, or on x-ray absorption spectroscopy.

SOFT CONDENSED MATTER PARALLEL SESSION

Organisers and Chairs: Stephan.V. Roth (User Organisation and HASYLAB), Christian Riekel (ESRF)

On 6 February 2008, the Soft Condensed Matter Parallel Session was held during the ESRF's User meeting. Organizers were Christian Riekel (ESRF Group leader) and Stephan Roth (HASYLAB/DESY Hamburg, Germany & Users Organization).

This year's parallel session had two objectives. First, to review the response from the user side of Soft Condensed Matter to the upgrade program, and secondly, to give an overview over selected long-term proposals in the soft condensed matter group. Hence the session was divided in two parts. In the first part Christian Riekel gave an update on the Soft Condensed Matter beamlines with special attention to nanobeams and high-throughput facilities. Afterwards, Patrick Davidson (University Paris Sud, France), representing the Programme Committee for the session on Soft Condensed Matter and Biopolymers chaired by Jean Doucet, gave a short overview over the results of the discussion on 23/24 October 2007 during the upgrade meeting.

The second part of the session was dedicated to external presentations of results of selected long-term proposals in the Soft Condensed Matter group. The first one was given by Oskar Paris (Max-Planck-Institute for Colloids and Interfaces, Potsdam, Germany). He showed, how microbeam SAXS & WAXS scanning investigations at ID13 and at the μ Spot-beamline at BESSY; Berlin, allow for mapping structural parameters. Furthermore, he put strong emphasis on real-time data evaluation to cope with the huge amount of data. The second presentation was given by Frederic Pignon (University Joseph Fourier, Grenoble). He reviewed his results on the structure of Casein micelle dispersions at ID2. Especially, he focused on in-situ SAXS during ultrafiltration which shows deformation of micelles near the membrane, leading to a decrease of the permeation flow. The third talk was given by Jean-Baptiste Salmon (LOf, UMR CNRS-Rhodia-Bordeaux 1, France). He presented experiments using microfluidic devices in combination with X-ray scattering. He proved, how to map in a combinatorial way the full phase-diagram concentration-temperature of a complex fluid using a multi-channel microfluidic device.

In summary, the session had around 40 participants. The division of the session into two parts was very well appreciated by the participants. Concerning the instrumentation, each of the long-term-proposal-presentations showed unique approaches to its specific research area. However, in common all speakers clearly expressed the need for supplementary in-situ techniques, as e.g. fluorescence, DLS.

X-RAY IMAGING PARALLEL SESSION

Organisers and Chairs: Laszlo Vincze (User Organisation and Ghent University), Eric Maire (INSA, Lyon, France & Users Organisation), José Baruchel (ESRF)

There was a steady number of about 30 attendees in the audience all through the 2 hours of the parallel session. The aim of the session was to give recent highlights presented by users and also to bring information for the user of the imaging group from the contacts at the ESRF. For this purpose, three speakers were invited from different fields of research using different imaging techniques and showed results obtained at the ESRF. Jose Baruchel, the head of the imaging group gave also a talk at the end of the session to inform users about the new aspects of the ESRF upgrade program.

The first invited talk was given by Tanya Smith and coauthors. Tanya showed us how they have been using X-ray tomography in the phase contrast mode to image teeth and fossils. These studies are extremely useful for our understanding of the human evolution. X ray tomography in the phase contrast mode is a unique technique for identifying the growth of the teeth. ID 19 is now widely seen as a leading facility and attracts more and more users in this area of research because it remains one of the only places in the world where these images can be performed. Tanya's presentation is a very good example of the magnificent results obtained in this field. One can anticipate a huge development in this area of research and this justifies the account for these applications in the upgrade program.

The second invited talk was presented by Guillermo Requena *et al.* The talk presented an application of the same techniques as the first talk, but applied in this second case to the understanding of the evolution of the microstructure of engineering materials. Although perhaps less appealing to a wider audience, this problem is important from the perspective of developing new materials. The talk was then more dedicated to materials science problem. It was shown that X-ray tomography is again a unique way of characterizing the percolation of a given phase in a microstructure. This requires more automatic quantification through image processing than in the preceding case where artifact retrieval and quality of the images is the important issue.

The last invited talk was given by Max Wilke *et al.* Although not used as a direct imaging technique in the present talk, it was shown in two different examples that X ray fluorescence both at the global and local scales performed on ID21 give useful information on the chemical state of different elements. The examples were all selected in the field of geology.

Jose Baruchel finally made an overview of the activities of the imaging group, of the proposals of the group for the upgrade and of the plans finally accepted by the SAC. It appears that imaging is concerned by four of the seven accepted new beam lines. Jose announced us a workshop to be held at the ESRF in November or December to help experts to go in more details into the plans for these new beam lines. The workshop will include a first day general presentation and a second day with two parallel workshops, one dedicated to the new NINA beam line (nano imaging, nano analysis) and the second to the IMPACT beam line. Users are going to be informed very soon and are asked to attend to bring their input. It is also time for users to try to lobby their government in order to help the ESRF Upgrade Project, and more in particular push the Peninsula project (a joint facility for all the imaging beam lines including microscopy at different scales) to be accepted in the near future (it is presently in the third priority of the first period of the upgrade). A web site is going to be available soon to help the users in this lobbying task.

X-RAY ABSORPTION AND MAGNETIC SCATTERING

Organisers and Chairs: Paolo Ghigna (University of Pavia, Italy & Users Organisation), Nick Brookes (ESRF)

The parallel session had four invited speakers. The talks lasted 20 minutes plus 5 minutes of discussion.

14.00-14.20: G. Aquilanti (ESRF): X-RAY ABSORPTION SPECTROSCOPY WITH MICROMETRIC SPATIAL RESOLUTION AND FAST ACQUISITION: A NEW TOOL FOR EARTH SCIENCES

14.25-14.45: C. Mazzoli (ESRF): COMPLETE POLARIMETRY OF X-RAY DIFFRACTION IN RESONANT REGIME: COMBINED TECHNIQUES TO SINGLE OUT MICROSCOPIC INFORMATION IN STRONGLY CORRELATED ELECTRON SYSTEMS.

14.50-15.10: M. Rovezzi (ESRF): X-RAY ABSORPTION FINE STRUCTURE APPROACH IN THE STUDY OF DILUTED MAGNETIC SEMICONDUCTORS

15.15-14.35: F. Duc (Laboratoire National des Champs Magnétiques Pulsés (CNRS-UPS-INSA) – 31400 Toulouse, France): SYNCHROTRON X-RAY EXPERIMENTS IN PULSED MAGNETIC

20 minutes of discussion on general issues concluded the session. The discussion mainly focused on the upgrade programme, with contributions from Nick Brookes and William Stirling. Francesco D'Acapito raised the question of the position of CRG beam lines in the framework of the upgrade programme.

HIGH RESOLUTION AND RESONANCE SCATTERING

Organisers and Chairs: Tullio Scopigno (University of Rome “La Sapienza”, Italy), Rudolf Rüffer (ESRF).

The parallel session was held on 6th February 2008 in the meeting room of the Control Room. The event, which attracted a significant number of participants (the room was fully packed) was based on 5 reports representing the different beamlines belonging to the HRRS area. The aim of these reports was to emphasize the state-of-the-art and the future needs of the scientific community in the context of the ESRF 2008-2017 Upgrade Programme.

The event was opened by a welcome speech by Rudolf Ruffer (ESRF) and a short introduction by T. Scopigno (University of Rome “Sapienza” and UOC), followed by the reports of the five invited speakers.

Daniele Fioretto highlighted the importance of the 0.1 meV resolution achievement for the area of High Resolution Inelastic X-ray Scattering, pointing out how this achievement would allow to bridge the existing gap with other technique such as Brillouin and Ultra Violet scattering, particularly relevant for the physics on Disordered Systems.

Alfonso San Miguel discussed host-guest interactions in nanointercalated materials studied using IXS as a local probe. He showed how these are at the origin of a number of attractive properties including superconductivity, thermoelectricity or enhanced mechanical stability. Specifically, he demonstrated how IXS can contribute to the study of the dynamics of silicon clathrates, comparing to other techniques probing the phonon- DOS. He also focused on a particular type of pressure induced phase transition, i.e. the isostructural homothetic volume collapse of silicon clathrate materials in the case of Ba₈Si₄₆.

Ralf Roehlsberger discussed how the future advances in the development of third-generation synchrotron radiation sources should allow to perform inelastic X-ray scattering experiments with energy resolutions in the micro-eV range, suggesting the necessary instrumental requirements and advancing a possible innovative experimental layout. He pointed out how this could open new avenues for the study of dynamics on mesoscopic length scales that determine the properties of artificially structured or self-assembled materials, presenting a selection of possible applications.

Moniek Tromp presented XANES data obtained on Au and Pt nanoparticles, providing detailed insights on reactant adsorption sites as well as on reaction mechanisms. She also offered an outlook into the planned developments of RXS for applications in homogeneous and heterogeneous catalysis.

Abhay Shulka gave a presentation on the future perspectives for the study on electronic excitations by means of Inelastic X-ray Scattering. His contribution was particularly timely as this topic is one of the flagships of the 2008-2017 ESRF Upgrade.