ESRF Users' Meeting 2007: reports from parallel sessions

MX PARALLEL 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 Spectroscopy around Biological Crystallography, held at the Institut de Biologie Structural, IBS. A session of presentations given by Edward Mitchell (ESRF) on ESRF Upgrades, by Joe Patel (Astex-Therapeutics) on the Impact of automation on drug screening/discovery and by Gordon Leonard (ESRF) on remote bean line access was concluded by a general discussion, animated by Sean McSweeney (ESRF), and mainly devoted to the ESRF long Term Strategy.

The main points of the discussion can be resumed as follows:

- The idea of substantial upgrading and the creation of an MX village have been well received - the question remains how this upgrade will take place and whether major logistic arrangements will have a disruptive effect on current MX operation. Unfortunately, no specific dates have been given in the Conceptual Design Reports.
- Current MX operations represent 45 % of the ESRF users visits. Given this large percentage and the increased scientific throughput obtained over last few years Macromolecular Crystallography should be considered as a main line of research activity at the ESRF – however, in the order to maintain a competitive edge, the upgrades proposed by the ESRF need to be revisited and complemented by constructive input form the MX users community.
- Interdisciplinary research around X-ray crystallography is certainly the way to go in the future– but choices have to be taken.
- Focus should not only be put on hardware, but as well on expertise and intellectual overview; an eye should be laid on developments carried out at other Synchrotrons. Build up local knowledge!
- A major focus should be put on spectroscopy methods: parallel recording of spectroscopic data during X-ray data collection, not only for kinetic measurements but as well for monitoring of radiation damage (EPR online, measurement of number of radicals generated??). If done routinely, it will attract users. Another priority is sample preparation on-site, for micro- and nano-spectroscopy issues. Off–line spectroscopy facilities could be advantageous for sample preparation. XANES measurements can give valuable information, could be straightforward and atomized; expertise is already on site.
- Protein SAXS: should ID14-3 dedicated fully or only half time to SAXS measurements?
- A better integration of Data Management with beam line software will be necessary..
- More training of local contacts and users will be required
- Preventive maintenance is a major issue: later start-up times could be advantageous.
- Detectors: pixel detectors would be of great benefit, if not absolutely necessary, for challenging experiments to be carried out in the future (ex. Biological imaging) – the question remains whether available financial resources are available.

SURFACE AND INTERFACE SCIENCE PARALLEL SESSION

Organisers and Chairs: Chris Lucas (User Organisation and University of Liverpool), Jorg Zegenhagen (ESRF)

This parallel session was held in a seminar room of the new Carl-Ivar Brändén Building which was an excellent venue. A packed room (as always!) was treated to 5 talks during the 90 minute session. Ivan Vartaniants (Hasylab at Desy, Hamburg, Germany) gave the first talk describing recent coherent GISAXS measurements of quantum dot samples that were obtained on ID1. He showed how individual quantum dot shapes could be reconstructed from the data. Marie-Ingrid Richard (C.E.A., Grenoble and ESRF, Grenoble, France) described how forbidden reflections could be used to study stacking faults in silicon presenting results obtained on ID1 and BM32. Edvin Lundgren (Lund University, Sweden) then presented some data obtained on the newly refurbished ID3 in which the structure and reactivity of a $Pt_{25}Rh_{75}$ single crystal catalyst was examined under realistic high pressure reaction conditions. Christian Kumpf (University of Würzburg, Germany) illustrated that the x-ray standing wave technique could be used to obtain high-precision structural information about large organic molecules adsorbed onto metal surfaces and previewed his upcoming experiments on ID32. Finally Jorg Zegenhagen (ESRF) gave an update/summary on the developments and achievements at ID1, ID3 and ID32 and described the opportunities for the wide range of surface and interface science experiments that can be performed now (or in the near future) at the ESRF. Unfortunately due to the shortness of the session there was no time for discussion of the ESRF long term strategy that had been presented to the users in the plenary session during the morning.

MATERIALS SCIENCE PARALLEL SESSION

Organisers and Chairs: Alain Lodini (User Organisation and Univ. Reims), Ake Kvick (ESRF)

Areas of materials science and engineering research in which synchrotron X-rays play a leading role are those identified as major socio-economic drivers, and which contribute strongly to the formation of a pan-European knowledge-based economy.

The meeting commenced with a brief presentation of recent developments by the relevant beamline scientists, in the areas of time-resolved diffraction, high-resolution powder diffraction, high-energy scattering, and high-pressure experiments.

We then received a presentation on the new microdiffraction station BM 32, where the beam dimension can be focussed down to submicron size. This new set-up is dedicated to the measurement of texture and strain in polycrystalline materials.

The meeting then focussed on four presentations from users in the areas of :

- Multi-scale analysis of shape memory materials
- In-situ studies using high-energy X-ray diffraction
- Application of high-energy X-ray diffraction to engineering components
- Time-resolved in-situ studies of complex structures with oxygen intercalation

The meeting was constrained by the time available, and the participants would have welcomed the opportunity for further discussion. 1h30 for a session covering the whole field of materials science and engineering is too short.
It was proposed to continue the discussions by email or Web. It would be better to have a longer session in the future user meetings.

SOFT CONDENSED MATTER PARALLEL SESSION

Organisers and Chairs: S.V. Roth (User Organisation and HASYLAB), C. Riekel (ESRF)

The parallel session of the Soft Condensed Matter (SCM) group was held on Wednesday, 07.02.2007, 14:00-15:30. It had a very active participation from the SCM beamlines as well as from the user community. The program was as follows. C. Riekel (group leader SCM , ESRF-ID13) gave a short introduction and overview over present status and future possibilities including the upgrade plan of SCM and ESRF. Martin Müller (University of Kiel, Applied Physics, Germany) presented the possibilities of in-situ stretching experiments on biopolymers with controlled hydration environments using micro- and nanofocused beams at ID13. Michel Cloitre (ESPCI-CNRS; Laboratoire Matière Molle et Chimie, Paris) presented his results on shear thickening in concentrated micellar solutions studied by Rheo-SAXS on ID2. In the second part, dedicated presentations of ID10A/B and ID2 were given. Oleg Konovalov (ESRF-ID10B) presented new sample environments at ID10B for studies of two dimensional bio-materials. Anders Madsen (ESRF-ID10A) showed low temperature sample environments at ID10.

A very active discussion was concerned the actual sample environment and trends at the various beamlines of SCM.

Concerning small beams in the nanometer range at ID13 it was pointed out, that this development requires high demands on mechanical and thermal stability. Furthermore, questions arose concerning the useable beam size and sample volume for scattering experiments. It was pointed out, that especially for in-situ stretching experiments special has to taken concerning stability of the stretched sample itself. Furthermore, it was agreed, that dedicated user workshops should be performed where users can give input and show their demands in this strongly developing nanofocusing field. Concerning ID10B, the use of high energies and small beams was very well accepted. Concerning ID10A, the low-temperature environment with 0.01K/h stability impressed the user community. Concerning ID2, it was asked if the Rheo-SAXS apparatus, showing excellent results, could be upgraded with a temperature control.

Further topics discussed were top-up-mode, high-throughput SAXS, and pixel detectors. Concerning the detectors, it was agreed, that 1000Hz frame rate, photon counting and a pixel size 12-50µm would be very useful.

To summarize, the main topics of interest showed the trends of future scattering experiments in SCM: small (nano) beams and high (reciprocal space resolution). More user workshops dedicated to small beams are needed to discuss and elaborate the trend in this field.

X-RAY IMAGING PARALLEL SESSION

Organisers: Laszlo Vincze (User Organisation and Ghent University), José Baruchel (ESRF)
Chair: Christian Schröer (Univ. Dresden)

The X-ray imaging parallel session featured three highlight talks reporting on user-experiments from various beamlines, and a short summary by the group leader (José Baruchel) concerning the various technical/methodological developments within the Imaging group as well as a report on the expected developments of X-ray imaging techniques in the framework of the Upgrade Programme.

The highlight user reports included the following topics.
Alexandre Simionovici gave an overview on experiments performed on beamlines ID22/ID21, devoted to high/low energy microspectroscopy studies, on comet coma particles returned to Earth within NASA's Stardust mission. Results were shown corresponding to a collection of 6 so-called keystone samples out of a total of 23 used in the study by several international teams. Terminal particles as well as fragmentation tracks in aerogel were mapped out with micron resolution, recording total mass composition for elements of Z=15 by means of X-ray fluorescence, as well as structural information by X-ray diffraction.

Luc Salvo reported results from in-situ fast X-ray tomography investigations of microstructural changes occurring during solidification and partial remelting of Al-Cu alloys. He pointed out that the understanding of some fundamental mechanisms in metallurgical science requires 3D visualisation of the material evolution during thermal treatment, which can be achieved only by performing in situ 3D tomography experiments at a spatial resolution of the order of few microns. The main constraint is the time duration of a complete scan (acquisition of radiographs over 180°) which needs to be less than 30s. Such high-speed tomographic acquisition is now possible at ESRF thanks to the high photon flux, the very fast cameras (DALSA or the latest FReLoN 2k) and the optimisation of the micro-tomograph set up at ID15 and ID19.

François Graner summarized their studies on the dynamics of liquid foams and their scale invariant regime. He showed results of high-speed X-ray tomography on liquid foams, which consist of bubbles of gas separated by a continuous phase of liquid occupying a small fraction of the foam's volume. The use of X-ray tomography at high speeds makes it possible to follow the foam evolution in time.

The subsequent discussion was introduced by a general report on the future evolution of X-ray imaging within the Upgrade Programme by J. Baruchel. His talk identified the highest priority developments and needs for the X-ray imaging community which are associated with the following areas:

1) Evolution of the biomedical work: improvements in biomedical (functional) imaging and developments in clinical radiotherapy within the framework of large collaborations for this type of cancer treatment.
2) Further evolution in microtomography and microspectroscopy should satisfy the following requirements:
    - more access to users
    - better spatial resolution down to nanoscopic levels
    - better temporal resolution

The reduced time (1.5 hours this year) devoted to the X-ray Imaging parallel session resulted in a too short discussion on the Upgrade Programme. In order to be able to assemble an attractive scientific programme for the X-ray imaging session which attract a sufficient number of users, and which can be coupled with a sufficiently detailed discussion, the duration of the parallel session should be increased to 2 hours.