

Report on BM30B/FAME May 17-18, 2005

This project was started in 1999, the beamline designed, constructed and commissioned by 2002 and commenced with scheduled users in September of that year. Dedicated to EXAFS and XANES, the scientific programme on FAME has concentrated on Environmental and Earth Sciences, Physics, Catalysis and Biology during the last two and half years. During this time the support team has been set up, comprising five permanent employees and two post-doc researchers employed by CNRS and CEA. Originally the technical emphasis of FAME was directed at determining atomic environments of elements at very low concentrations in natural systems. Subsequently the beamline operations have been streamlined and made very efficient to accommodate a wide range of other measurements and versatile experiments, of which more than half now involve in situ environment stages (cryostat, HP and HT cells, catalyst rigs etc). An extensive user manual has been produced and formal training sessions for users set up. Our impression is that FAME has developed into a very reliable and user-friendly facility offering a very stable focussed beam from 4 to 22 keV, with unfocussed beams available to 40 keV. For X-ray spectroscopy this encompasses most of the periodic table relevant to environmental and biological science and with the X-ray detectors available concentrations that are realistic. Finally we note that the user community has developed from researchers mainly from the Grenoble region to now include the majority of French groups in environmental and earth science, reflecting the objectives of the original funding from CNRS, CEA and the Rhône-Alpes Region.

Research by Users

Since it was established in 2002, FAME has attracted an extensive range of science. We are particularly impressed by the work on heavy metals, their speciation, toxicity and remediation. In the process they have developed a powerful finger printing methodology for analysing complex mineralogical and biological systems from a X-ray spectroscopy data bank of model systems. This has been applied to contaminated sediments, soil-root systems, ground waters, colloids, cements, slags and ash. Across this wide portfolio there is also an imaginative integration of approaches from the molecular scale to the macroscopic level encountered in environmental hazards. We highlight the phytoremediation of metal polluted soils by Sarret (LGIT) and the microbial

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sequestration of As in Bangladesh rivers and groundwaters by Rose (CEREGE), both benefiting from the very stable EXAFS conditions on FAME. The work of Arcovito (Stockholm) and Della Longa (L'Aquila) on photolysis of myoglobin systems has exploited the ultra dilute capability of the CRG in resolving subtle conformational changes from high quality XANES spectroscopy.

Elsewhere in the areas of nuclear fuel, catalysis etc we judge that the experiments developed so far are of high standard.

Research by Staff

The panel found the work by Hazemann on supercritical liquids and the precipitation from solutions under these extreme conditions outstanding. On the one hand the engineering of HP/HT cells with spherical Be windows has resulted in reliable operation under these taxing conditions, which is typical of the high level of technical developments on FAME. On the other hand the performance of the XAFS facilities has meant that very precise analysis has been possible of density, solubility, transport properties and the extraction of metals with implications for ore deposits and pollution containment. This pioneering work has attracted groups from France (Toulouse, Lyon, Paris) and more recently Australia, a good example of the enlargement of the user base but which is currently inhibited by present staffing levels.

Overall we consider the average activity is high and that the technical developments are in many cases exceptional. Nevertheless we recommend:

- the successful technical networking established between FAME and local laboratories, including the ESRF be further developed
- with the maturation of the beamline attention be given to increasing publications from FAME which do not in our view reflect the scientific success of this attractive beamline

Technical Status of the Beamline

This new beamline has benefited from improvements in X-ray optics, detector design and beamline control. Despite this we consider that the FAME team has achieved more than best practice for a 3rd generation source and has delivered a first rate XAFS facility well-suited to the environmental and earth science community in particular. The introduction of a user training programme is applauded, as is the creation of a comprehensive user manual.

Future Technical Developments

Given that this is a new beamline with excellent performance, it is good to see a programme developing for refining the beam optics and X-ray detection to meet future scientific challenges. In particular we strongly support the following initiatives:

- incorporation of digital electronics into the 30 element Ge fluorescence detector system. This will enhance the count rate by a factor 3 and create a unique capability at the ESRF.
- development of a microfocus KB mirror assembly to perform EXAFS for energies 4 – 22 keV with a spatial resolution of $20 \times 20 \mu\text{m}^2$ which is a prerequisite for analysis using diamond anvil cells and other HP/HT devices.
- implementation of spherically bent analyser for selection of fluorescence of minority species with an energy resolution of 20 eV, sufficient to remove unwanted Compton Scattering and fluorescence contamination from host matrix.

Future Scientific Directions

Whilst the current scientific programme is positively organised and very productive in the first 2 to 3 years of user operation, we suggest that FAME may encounter challenge in remaining leading-edge if attention is not paid to prioritisation and identification of future opportunities.

- We think that the whole field of supercritical systems is a burgeoning area, not just for earth science applications but in enriching fundamental physics and chemistry of heterogeneous complex systems involving liquids. With the technical lead that they have established we believe that FAME is now well-placed to become a scientific reference in this field. For this they are encouraged to establish this as a new theme for FAME, in addition to environmental science. For this they will need to strengthen their collaborations and dedicated manpower in this area.
- Similar experimental arrangements and tools could also be harnessed to explore the diversity of micro organisms in extreme environments. The ability to record XAFS at very dilute levels, detect density and chemical environment in living systems, coupled with the facility of robust environment stages capable of controlling and changing pH, T, P, redox, salinity etc we believe will give FAME an international advantage in this exciting field. We also recognise that this should pay dividends in future environmental science applications.

Staff

We recognise that huge efforts have been made by the existing FAME team since 2002 but that the future success of this beamline will require some additional support.

We recommend that:

- The engineer due to retire is automatically replaced to support electronics and computing
- an additional scientist is recruited to assist in promoting the scientific potential of the FAME beamline

Summary of Recommendations

From this strong and successful initial phase of FAME we would recommend:

- they build on the environmental studies and in situ experiments to extend the visibility of FAME to a wider community
- they take the opportunity to enlarge the user community of FAME to other non-French research groups making use of the special developments made in the robust monochromator and detector design
- consideration be given to the level of in-house support. Currently there are two dedicated staff for scientific and technical assistance which we consider insufficient to fully exploit the scientific capabilities of FAME

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