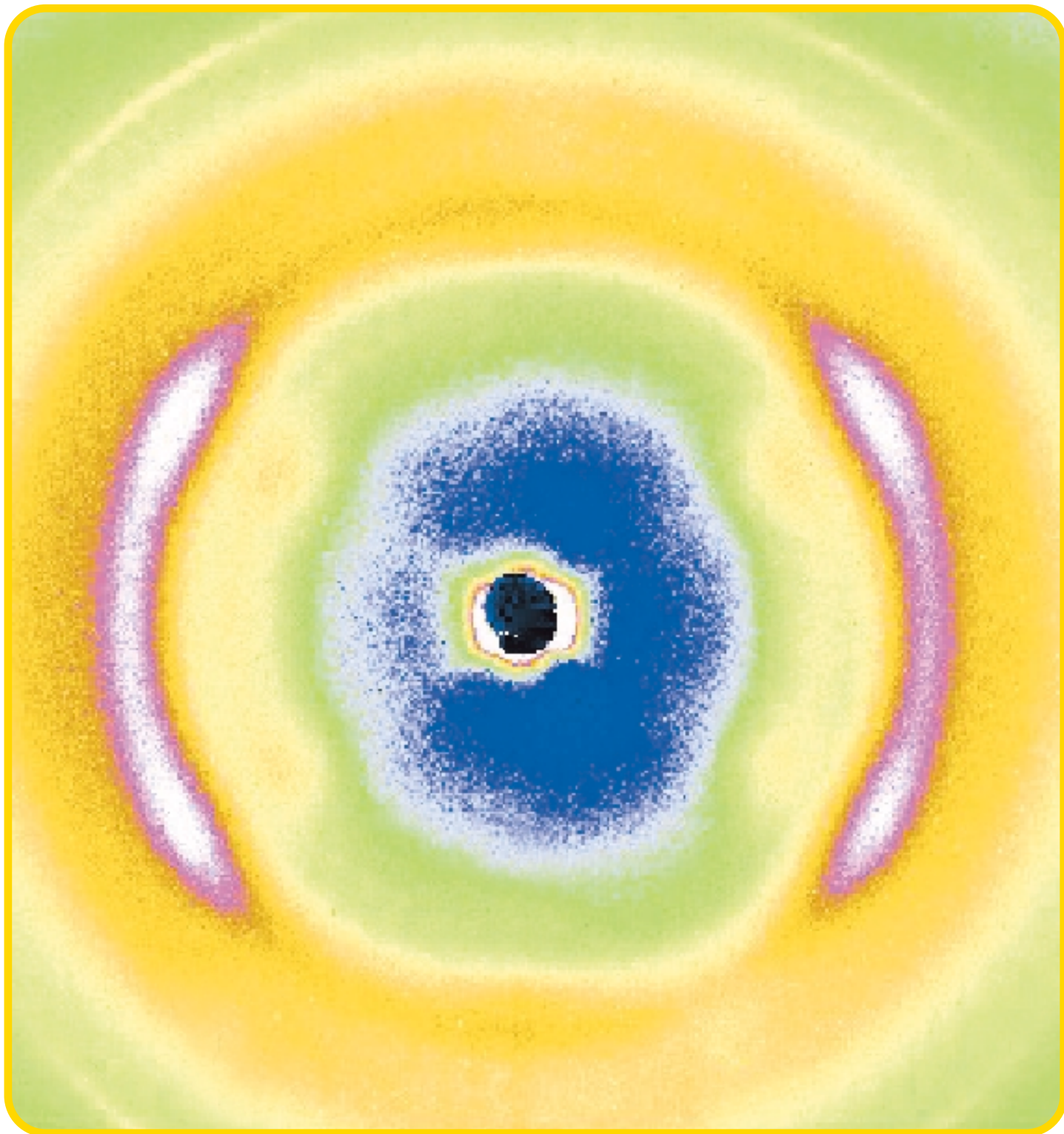


ESRF NEWSLETTER

EUROPEAN SYNCHROTRON RADIATION FACILITY

November 2002 - N° 36



ISSN 1011-9310



THE NEWS MAGAZINE OF THE ESRF

<http://www.esrf.fr/UsersAndScience/Publications/Newsletter>

Contents

HIGHLIGHTS	Austria Joined the ESRF - page 2 Czech Participation in the ESRF Continued - page 2	WORKSHOPS AND CONFERENCES	Fibers and Polymers - page 5 Highly Correlated Electron Systems (HCES) Studied with Synchrotron Radiation Techniques - page 5 Surfaces and Interfaces on the Atomic- and Nano-Scale: Semiconductors, Magnetic Materials and Oxides - page 6 Complementary Methods in Structural Biology - page 6 Aussois - page 9 The 7th X-ray Microscopy Conference - page 9 Crystal Chemistry - page 11 X-TOP - page 11 Polymer Workshop for Industry - page 16 Three-way Meeting - page 18 X-Ray Optics Workshop - page 18 Accelerator Reliability Workshop - page 25
EDITORIAL	By W.G. Stirling, Director General - page 3		
NEWSLETTER IN BRIEF	Users Meeting and Satellite Workshops - page 4 36th and 37th Meetings of the ESRF Council - page 7 Operation with Users in 2001 - page 8 The 12th Session of the HERCULES Course - page 10		
NEWS FROM THE EXPERIMENTS	Selected Scientific Highlights - page 12 News from the CRGs - page 17 FAME38 at ILL/ESRF - page 19 The Partnership for Structural Biology: A European Centre of Excellence - page 20		
NEWS FROM THE MACHINE	Future X-ray Facilities - page 22		
EUROPEAN COLLABORATIONS	Collaboration with EIROFORUM - page 26 European Round Table - page 27		
EVENTS	Tenth Anniversary of the Beam - page 28 New Directors - page 28 CD-Rom "Exploring matter with synchrotron light" - page 28		

Highlights

AUSTRIA JOINED THE ESRF (1 JANUARY 2002)

The Austrian Academy of Science (ÖAW) and the ESRF agreed that the ÖAW would become a Scientific Associate of the ESRF at a level of 1% from 1 January 2002. A medium-term

arrangement, which came into effect on 1 January, enables Austrian scientists to carry out experiments at the ESRF under the same conditions as scientists from Contracting Party Countries. The formal

signing of the arrangement concerning the long-term scientific use of the ESRF by Austria is planned to take place on 5 December 2002.

CZECH PARTICIPATION IN THE ESRF CONTINUED

Dr Jungwirth, new Director of the Institute of Physics of the Czech Academy of Science (FZU), visited the ESRF on 19-20 September 2002. In his capacity as Director of the FZU he is

responsible for the Czech involvement in the ESRF. After constructive discussions concerning an adjustment of the Czech participation to correspond more closely to their actual use of the ESRF's

facilities, Dr Jungwirth agreed to an increase of the Czech participation from its current level of 0.35% to 0.38% in 2003 and 0.41% in 2004.

EDITORIAL

Since the last ESRF Newsletter, we have seen a number of changes among our senior staff. I would like to thank particularly four colleagues who have left recently.

Christof Kunz has been associated with the ESRF since the idea of a European synchrotron radiation source was first proposed; he was a member of the ESF working group, formed in 1976 and chaired by H. Maier-Leibnitz, which produced the famous 1977 "Black Book". Since that time, Christof has been involved with the ESRF in many different roles, culminating in his period as Director of Research between 1995 and 2001. We are very grateful to him for all of his work in support of the ESRF. But Christof continues with his association with ESRF since he is currently working again as an experimental physicist on the extension of photoemission techniques to higher photon energies.

After eight years of service to the ESRF **Tony Davies** retired as Director of the Administration at the end of January. His lively interest in and his continued support for the scientific programme is well known. Under his guidance the ESRF administration developed into the efficient yet friendly and informal service that we know today.

A few months later **Peter Lindley** returned to the United Kingdom after five years as Director of Research. Peter oversaw the completion of the ESRF's portfolio of thirty beamlines, with a particular attention to the development of macromolecular crystallography. Due to his insight and rigour, the ESRF is now one of the world's leading centres for research in this vital area. Peter also tirelessly

worked towards the realisation of the Partnership for Structural Biology (PSB), to which I will return below.

Finally, **Bill Thomlinson**, Head of the team on the Medical Beamline, is leaving to assume the responsibilities of Director of the new Canadian Light Source. Working with colleagues from the ESRF, the Centre Hospitalier Universitaire de Grenoble, the University of Helsinki, and other centres, Bill has provided the ESRF with an outstanding synchrotron facility for medical imaging and microbeam therapy.

We are very grateful to Christof, Tony, Peter and Bill for their many crucial contributions to the ESRF and we wish them well in their new careers or pursuits.

Our major construction project at the moment concerns the new ID23 beamline complex for advanced structural biology. This is the ESRF's largest contribution to the exciting Partnership for Structural Biology. After almost 18 months of discussion, argument and debate this virtual partnership will become reality in mid-November when the agreement uniting

the four partners will be signed. We are delighted that ESRF, ILL and the EMBL Grenoble outstation will be joined in the PSB by the IBS (Institut de Biologie Structurale), one of France's leading life science research centres. The IBS, which is a joint CEA-CNRS-UJF laboratory, will bring valuable expertise in NMR and other related techniques to complement the biochemical, X-ray and neutron diffraction expertise of the other three partners. The PSB is described in more detail in a special article in this Newsletter.

Further details of the ESRF's current projects and future plans can be found in the articles on the activities of the Experiments Division.



B. Thomlinson



P. Lindley



T. Davies and C. Kunz

This edition of the Newsletter also includes reports on February's Users' Meeting, recent workshops and the Council Meetings of last November and June. We also report on the outstandingly efficient operation of the Machine, statistics and major issues concerning the User Office, the ESRF's contribution to the HERCULES course, and information from the CRGs. Finally, our participation in projects involving the EIROforum (the collaboration between seven of Europe's leading intergovernmental research organisations) is presented, and we consider future events at ESRF.

I hope that you enjoy reading our Newsletter – there's something for (almost) everyone. We welcome your feedback and advice on new items for inclusion.

W.G. Stirling
Director General

USERS' MEETING AND SATELLITE WORKSHOPS

13 February 2002



L. Margulies receives the Young Scientist Prize from the hands of A. Fontaine.

This year, the Users' Meeting plenary day attracted some 330 participants from Europe, the USA and Canada, and as far as Brazil. Keynote lectures by G. Materlik and G. Sawatzky, and highlight talks by A. Yonath and H. Poulsen filled the morning session. This was followed by

lunch in discussion groups organised to present the new group structure within the Experiments Division. Ideas and suggestions from users arising from discussions were then outlined and debated briefly with ESRF management in a panel session following lunch.

The meeting was also an opportunity for the Hungarian Academy of Science, represented by its Secretary General, N. Króó, to sign an arrangement to allow scientists from Hungary to continue to use facilities at the ESRF.

A moment keenly awaited in the afternoon was the announcement of the winner of the Young Scientist prize by A. Fontaine, chairman of the award committee. This year's prize-winner, Lawrence Margulies, presented his work under the title "3D resolved



From left to right: J.-L. Plantier, acting Director of Administration, W.-G. Stirling, ESRF Director General and N. Króó, Secretary General of the Hungarian Academy of Sciences.

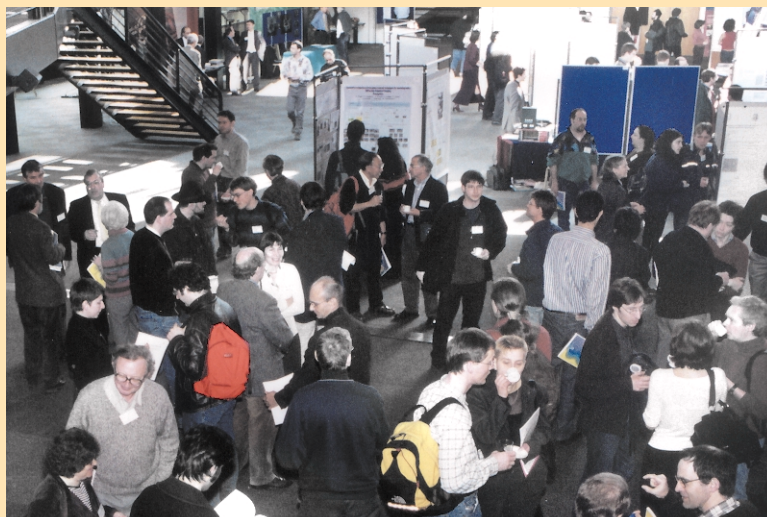
studies of plastic deformation in metals".

The talk was followed by a lively poster session, where some 80 posters were on display. An innovation this year was the award to the best poster. This was made by the Users' Organisation during dinner in the evening, to F. Demmel, S. Hosokawa, S. Pilgrim and M. Lorenzen, for their poster entitled "Optic modes in molten NaCl".

Satellite Workshops to the Users' Meeting

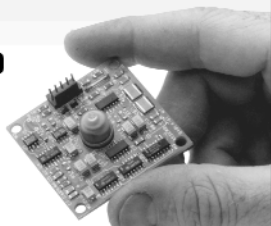
There were this year four satellite workshops to the Users' Meeting during which very interesting talks were given, which led to lively discussions.

Poster session



FIND ANGULAR POSITION WITH EASE AND PRECISION

**GRAVITY REFERENCED
INSTALL ANYWHERE
UP TO $\pm 60^\circ$
OPERATING RANGE**



Our precision tiltmeters give you new abilities to measure the angular movement and position of:

- Antennae
- Lasers
- Telescopes
- Foundations
- Any machine or structure

Use to find level, measure static tilts or determine pitch and roll. Choose from our:

- 500 Series – nanoradian resolution
- 700 Series – microradian resolution
- 900 Series – 0.01 degree resolution

Distributor: Sobetra Automation
Tel. 02/331.13.37, Fax 02/331.01.17, sobetra@arcadis.be
Langeveldpark Lot 10, P-Basteleusstraat 2
1600 ST-PIETERS-LEEUEW, Belgium

APPLIED GEOMECHANICS
Tel. (831) 462-2801 • Fax (831) 462-4418
applied@geomechanics.com • www.geomechanics.com

FIBERS AND POLYMERS

11-12 February 2002

Ninety-two participants – sixty-two of them from outside – attended this workshop which was held at the ESRF. The goal of the workshop was to bring together the polymer and biopolymer communities using synchrotron based experimental techniques on a common platform. Many participants felt it was a unique platform indeed.

The topics ranged from polymer colloids to solid polymers and fibrous biopolymers. This year's novelty in biopolymers was hagfish slime, which appears to form stronger fibers than spider silk. The majority of results were obtained by

wide- and small-angle X-ray scattering although a number of complementary methods like neutron scattering and photon correlation spectroscopy were mentioned.

The diversity of topics induced a number of interesting discussions between fans of particular techniques

and beamlines, which were continued amongst the 29 posters during the dinner-buffet in the ESRF entrance hall. The workshop concluded with a visit to the ID2 and ID13 beamlines, which gave attendees the occasion of discussing their pet-project with the beamline staff.



HIGHLY CORRELATED ELECTRON SYSTEMS (HCES) STUDIED WITH SYNCHROTRON RADIATION TECHNIQUES

11-12 February 2002

This workshop held in the ILL Amphitheatre was organised by P. Carra, F. Sette (Science) and A. Maden (Administration).

A list of 16 invited speakers from Europe and the USA attracted a registration of 85 participants. The programme included six sessions of seminars, which were delivered by the invited speakers and took place over two full days.

General Talks (M. Rice, Zurich; GA. Sawatzky, Vancouver), Ab-initio calculations (OK. Andersen, Stuttgart; W. Pickett, Davis; H. Ebert, Munich), Non-Fermi liquids - 3d transition metals (N. Bernhoeft, Grenoble; P. Bruno, Halle; M. Altarelli, Trieste), Vanadium Sesqui-oxide (F. Mila, Lausanne and S. Di Matteo, Grenoble), Synchrotron radiation techniques (J. Goulon, Grenoble; D. McMorow,

Roskilde; N. Brookes, Grenoble), High-Tc superconductors and fullerenes (Z-X. Shen, Stanford; M. Sigrist, Zurich, E. Koch, Stuttgart).

A number of posters were submitted and the following people were invited to give selected short talks: C. Dallera (Milan), M. D'Astuto (Grenoble), R. Przenioslo (Grenoble), A. Rogalev, (Grenoble) and J. Roehler, (Koln), LH. Tjeng (Cologne).

A pleasant workshop dinner took place at the Novotel in the centre of Grenoble, which provided a forum for less formal discussions.

The HCES Workshop was promoted alongside the ESRF by the SRRTNet, The Global Synchrotron Radiation Research Theory Network, and was funded by the European Union.



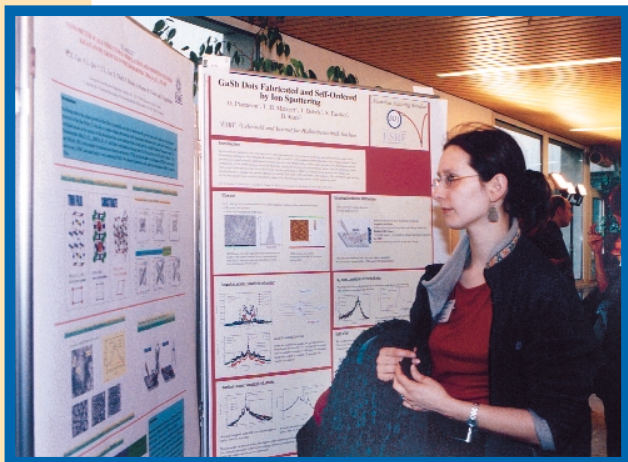
SURFACES AND INTERFACES ON THE ATOMIC- AND NANO-SCALE: SEMICONDUCTORS, MAGNETIC MATERIALS AND OXIDES

14-15 February 2002

The workshop was organised by J. Zegenhagen, N. Brookes, S. Ferrer, T. H. Metzger (science) and U. Ramseger (administration). An excellent panel of invited speakers

had attracted a total of 129 registered participants from 15 nations. It was evident that surfaces and interfaces on the atomic- and nano-scale are still in the focus of interest. The workshop was arranged in five sessions, four of them oral: two sessions on magnetic materials, one on semiconductors, one on oxides, and one poster-session, for which three timeslots on Thursday and Friday had been reserved. The workshop started with an impressive presentation by S. Parkin (IBM, USA) on nano-structured, magnetic (spin) memory devices, spanning the range from basic physics to application.

The ILL Chadwick Theatre was fully occupied from the beginning and listeners had to accommodate themselves on the stairs for this and several other highly popular talks. After lunch, about 40 admirable posters stimulated dynamic discussions, with the poster session being continued Thursday evening and Friday after lunch. The programme of the workshop finished with the presentation of the Best Poster Award (consisting of a corresponding document, a cheque, and six splendid ESRF Experiments Division mugs) to R. Roehlsberger (Rostock, Germany). Finally, about 30 participants could discuss and chat leisurely while attending a good dinner in a comfortable atmosphere at the restaurant Pique Pierre in St Martin Le Vinoux.



COMPLEMENTARY METHODS IN STRUCTURAL BIOLOGY

14-15 February 2002

Researchers from a wide range of scientific disciplines attended this workshop held on 14 and 15 February. The workshop examined the techniques available to the researcher interested in biological problems.

The meeting was opened by P. Lindley who, after describing the ESRF and its evolution, linked together the many techniques that must be employed in "problem-driven research". Sessions held on the first day were devoted to X-ray and neutron diffraction, Nuclear Magnetic Resonance (NMR) and electron microscopy. The second day was devoted to solution scattering techniques using both X-rays and visible light, synchrotron radiation circular dichroism and X-ray microscopy, finishing with an overview of the current status of

computer modelling of protein structures. Finally examples were given of the extra insight obtainable by the use of complementary methods in a scientific investigation. The meeting was brought to a conclusion by R. Fourme (Soleil) who drew together themes of the workshop and emphasised the importance of

synchrotron radiation to the field of structural biology. The workshop brought together a new group of scientists to the ESRF, most of whom were on their first visit to the ESRF, and emphasised the need for the scientists to employ all the techniques at their disposal in order to understand the complexities of biological systems.



36TH AND 37TH MEETINGS OF THE ESRF COUNCIL

held on 26/27 November 2001 and 4/5 June 2002

Scientific Programme

The Council noted the **Medium-Term Scientific Programme** for the period 2002 to 2006. This programme indicates as high-profile fields: Structural Biology, High Resolution Electron Spectroscopy, Very Large Magnetic Fields, Microfocus, Nanotechnology and Materials Engineering. The policy of continual enhancement/development of the machine and the experimental facilities is maintained. The programme also deals with the organisation of manpower and the need for a further building.

The Council also noted the progress in the preparation of the **Partnership for Structural Biology**, and authorised the Director General to sign the Memorandum of Understanding with EMBL, ILL and IBS, with the provision that a more detailed document will be submitted to the Council within two years.

Scientific "Juste Retour" (Fair Return)

The Council took note of the current scientific "juste retour" situation which continued showing an over proportional use by the Nordsync community. It noted that, in accordance with the "Resolution on corrective measures" adopted in June 2001, the Nordsync consortium will make an additional contribution to the 2003 budget over and above its pro rata share in the budget of 2003, the amount being 0.73 % of the totality of Members' contributions. In addition, the Council requested the Director General to report, at the next meeting, on measures to improve the situation of the under-balanced countries.

Scientific Partners

The Council

- approved an extension by a further two years of the arrangement on the medium-term use of the ESRF with the **Hungarian Academy of Science** (i.e. from July 2002 to June 2004),
- approved the conclusion of an arrangement on the long-term use of synchrotron radiation with the **Austrian Academy of Science** (i.e. from January 2002 to December 2006),
- authorised the Director General to

undertake negotiations with the appropriate legal body in Portugal with a view to an extension of the arrangement with the **Government of Portugal** (or to the conclusion of a new arrangement under similar terms with an organisation acting on behalf of the Portuguese scientific community), and recommended that the arrangement, once unanimously approved by the Council, should be signed on behalf of the ESRF by the Director General and the Chairman of the Council.

Financial and Procedural Matters

The Council

- approved that the **Purchasing Committee business** shall continue to be handled by the Administrative and Finance Committee;
- approved the **final accounts for the financial year 2000** and discharged the former Director General with respect to the implementation of the budget for 2000;
- noted the **second revision of the 2001 budget** (including the transfer of the posts of the Experimental Hall Operators from the Experiments Division to the Safety Group);
- approved the **budget for 2002** as presented by Management, providing for expenditure of 70 938 k in payments and requiring Members' contributions of 63 451 k ;
- took note of the **Medium-Term Financial Estimates (2003-2007)** presented by Management and confirmed 64 720 k as the planning figure for new contributions from Members to the budget for the year 2003, with due reservations about the availability of these funds.

Appointment of Chairpersons and Committee Members

The Council

- elected R. Feidenhans'l (Denmark) as Vice-Chairman of the **Council** for 2002 and 2003;
- appointed J.L. Martinez (Spain) as Chairman of the **AFC/AC/PC** and M. Steinacher (Switzerland) as Vice-Chairman of the **AFC/AC/PC** for the period from 1 July 2002 to 30 June 2004;
- noted the nomination of A.J. Ryan (Dept. of Chemistry, Univ. of Sheffield) as member of the **Science Advisory**



Since 1 January 2002, the ESRF Council has been chaired by R. Comès, who succeeded P.E. Zinsli. Robert Comès, 65, is solid state physicist and has worked both with neutrons and X-rays. From 1990 to 2000 he has been Director of LURE. His relationship with the ESRF dates from the ESF ad-hoc committee in the early eighties and AFC chairmanship during the ESRF Foundation Phase. Over many years he has been member of the French delegation to the ESRF Council. New Vice-Chairman is Robert Feidenhans'l (Head of the Material Research Department of the Risø National Laboratory).

Committee for the period up to the end of 2002, replacing D.I. Stuart (who had become member of the UK delegation).

Director of Research

Restarting the selection and appointment procedure for a Director of Research (succession of P.F. Lindley), the Council specified that

- the scientific orientation of the candidates looked for was "Structural Biology",
- a continuation of the future Director's research activities to a limited extent was acceptable,
- the first phase of the procedure (search for candidates and shortlisting) was to be organised by a small group made up of Council Chairman, Vice-Chairman, Director General and Council Secretary, aiming at having the interviews be held before the next meeting of the Council in November 2002.

The Council noted that, for the time being, F. Sette alone was leading the Experiments Division.

K. Witte

OPERATION WITH USERS IN 2001

During the year 2001, the full complement of 30 ESRF beamlines, together with 8 Collaborating Research Group beamlines (CRGs) were open for user experiments, the CRGs making 1/3 of their beam time available for general ESRF users. For the purposes of

scheduling experiments on beamlines, 2001 was divided into two periods, February to July 2001, and August 2001 to the User Meeting in February 2002, with run periods of six to seven weeks, broken by shutdown periods for installations, commissioning and maintenance.

Scientists requesting beam time submit applications for two deadlines – 1 March and 1 September - each year. For the proposal rounds in 2001, all 1582 applications for beam time were successfully submitted electronically. The increase in requests for beam time since 1997 is shown in **Figure 1**. It is to be noted that although the main beamline construction effort was complete by 1999, requests for beam time continue to rise, and totalled 24824 shifts in 2001. In the past, requests for beam time have outweighed the beam time available for allocation by roughly a factor of two. This pattern continued in 2001, when 11 281 or slightly more than 45% of the shifts requested were allocated beam time.

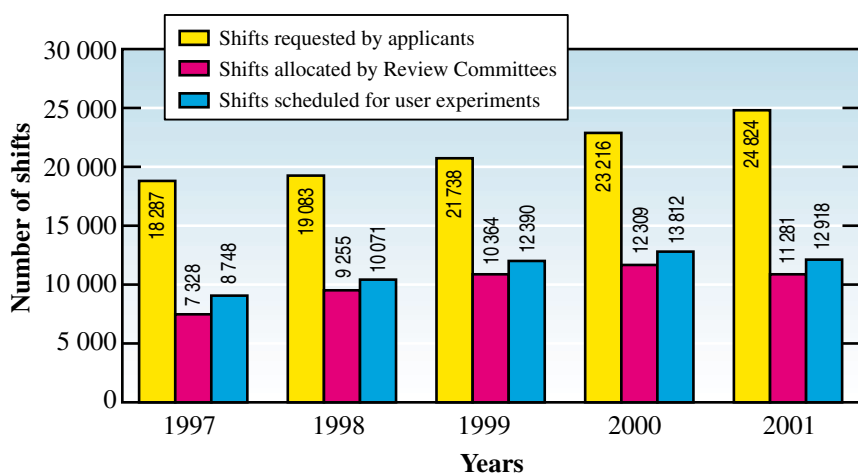


Fig. 1: Details of shifts requested, shifts allocated beam time, and shifts scheduled for user experiments, per year, 1997 to 2001.

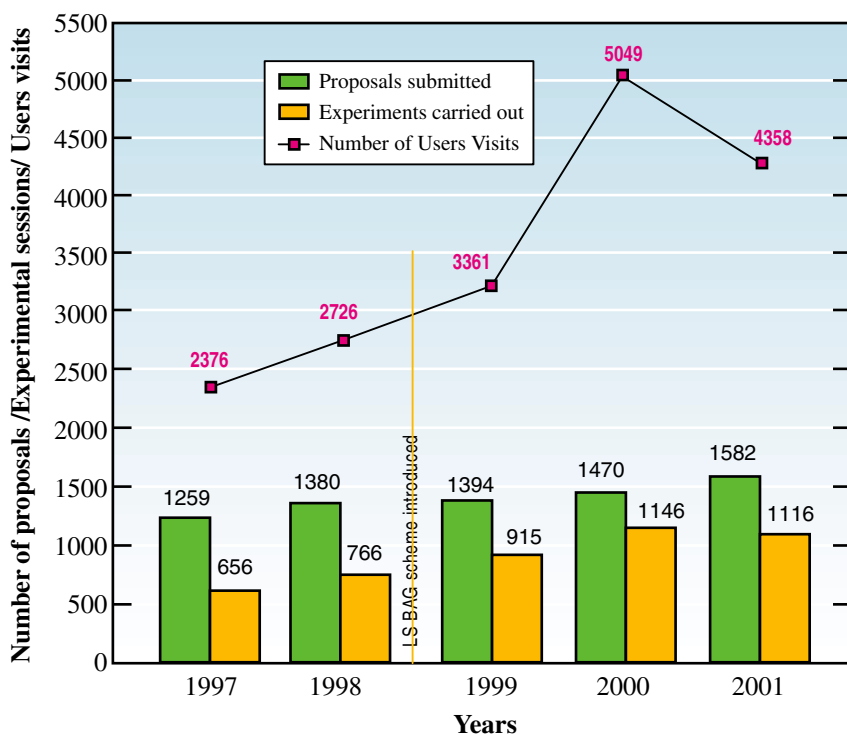


Fig. 2: Numbers of applications for beam time submitted, experiments carried out, and user visits, 1997 to 2001.

Experimental Programme

Concerning the experimental programme, the number of experimental sessions compared with number of applications for beam time over the scheduling periods from 1997 can be seen in **Figure 2**, which also shows the increase in the number of visits by users. The year 2000 saw a sharp increase in the number of user visits, with a total greater than in 2001. This peak is due to a slightly longer scheduling period, and correspondingly higher number of experimental sessions and user visits.

The breakdown of shifts scheduled in 2001, per scientific area, is shown in **Figure 3**. One of the features of this period has been the increasing number of projects concerned more with applied than basic research in materials science, engineering and environmental matters. As seen in **Figure 3**, experiments in these areas accounted for 11 % of the total number of experiments carried out in 2001. In addition, the number of macromolecular crystallography experiments has risen notably, due to a combination of the availability of five experimental stations dedicated to these projects, very rapid data collection times – frequently less than one shift –



AUSSOIS

22-24 May 2002

The third Experiments Division Science Days were held from 22 to 24 May, in Aussois and were attended by approximately 180 people. As for the previous meetings, the aim was to provide an opportunity to the scientific staff to reflect on the past and to discuss future perspectives. In the spirit of the new division structure, each scientific group was allocated a time slot of typically 1h30, in which, following a general introduction (in most cases by the current Group Head), recent research highlights were presented. These included as well work from the collaborative research groups (CRG). The two extensive poster sessions were preceded by poster clips in

which the PhD students introduced their work. A lot of effort and care was put into these posters and made the assignment of the best PhD poster award a very difficult task. The meeting was held in a very relaxed atmosphere catalysing many animated discussions, especially during the free afternoon where the bad weather kept everybody together under the roof of the Paul Langevin Center. The general feeling was that the Science Days are stimulating and essential for the scientific life of the Experiments Division, and the next meeting should be foreseen for fall 2003.



Surfaces and Interfaces	10 %
Chemistry	11 %
Hard Condensed Matter: Elect. & Magn. Properties	13 %
Hard Condensed Matter: Structures	18 %
Materials Eng. & Environmental Matters	11 %
Life Sciences	18 %
Methods and Instrumentation	6 %
Soft Condensed Matter	9 %
Others:	
Training, feasibility tests, proprietary research	4 %

Fig. 3: Shifts of beam time scheduled for experiments in 2001, by scientific area (total shifts 12918).

and the very successful operation of the Block Allocation Group (BAG) scheme. The number of BAGs, initially 20 late in 1998, rose to 38 by the second scheduling period in 2001. Furthermore, to cater to the experimental needs of a wide diversity of research projects, beam deliveries to the stations in 2001 were made in a variety of modes:

- multibunch (2 * 1/3 and uniform filling) - 64%
- hybrid mode - 5%
- 16-bunch fill - 23%
- single-bunch fill - 8%.

Next Deadline for Proposals:
1 March 2003

Finally, interested readers are reminded that deadlines for proposals for beam time are 1 March and 1 September each year. Further details are available on the Web at <http://www.esrf.fr>.

R. Mason

THE 7TH X-RAY MICROSCOPY CONFERENCE

28 July - 2 August 2002

The 7th X-ray microscopy conference was hosted by the ESRF from 28 July to 2 August. The X-ray microscopy conferences are held every three years and are the primary international forum for the presentation and discussion of advances in high-spatial-resolution X-ray imaging and its applications across a broad range of sciences. XRM2002 was held at the ATRIA World Trade Centre in Grenoble and was jointly supported by the ESRF, LURE and SOLEIL.

In addition to providing the latest information on the X-ray microscopy technique, the programme was set to emphasise scientific accomplishments from various fields such as Biology, Earth sciences, Materials Science, and Environmental Sciences.... The meeting attracted 239 participants from 18 nations (138 (from Europe), 48 (USA) and 53 (Asia)). Both the participation of 50 registered PhD students and the submission of more than 190 abstracts confirmed the rapid growth of the X-ray microscopy community.

On Wednesday afternoon, more than 120 persons participated in a 2-hour guided tour of the ESRF and visited several beamlines (ID13, ID19, ID21, ID22, and BM5). Thursday evening the delegates enjoyed a boat trip on the Lac du Monteynard prior a dinner at the "Chateau d'Erbelon".

The conference ended with the presentation of the Werner Meyer-Ilse Memorial Award, which is made to young scientists based on their contributions to the development of X-ray microscopy through either technical advances or applications. The winner was M. Feser, from Stony Brook University of New York, USA (see picture).



From left to right: A. Michette (King's College London, UK), chairman of the Werner Meyer-Ilse Award Committee, the award winner M. Feser (Stony Brook University of New York, USA) and Andrea, wife of the late Werner Meyer-Ilse.

THE 12TH SESSION OF THE HERCULES COURSE

from 17 February to 28 March 2002

During the six-week period from 17 February to 28 March, 2002, Grenoble hosted the HERCULES course (Higher European Research Course for Users of Large Experimental Systems). This school was funded through resources provided by the European Commission, the French Ministry of Education and Research, the national institutions CNRS and CEA, and two European large facilities, ESRF and ILL. The school is organised by the Grenoble Universities (UJF, INPG), the Université Paris-Sud XI, and several large facility centers (ESRF, ILL, CNRS, CEA, LURE, LLB) and is dedicated to the use of "neutron and synchrotron radiation" and continues to attract a large number of scientists: 66 full-time and 7 part-time participant, out of 93 applicants, took part in the 12th session. This year the selected PhD students and post-doctoral scientists came mainly from the European Community, but also from Eastern Europe (Poland, Czech Republic, Hungary, Turkey, Romania...), from the Americas (USA, Argentina) and from Asia (there was an agreement for the participation of 5 scientists from Taiwan).

Participants attended lectures, tutorials and practicals. The lectures, given by more than 60 speakers, top specialists in each field concerned, covered the various properties of neutrons and synchrotron radiation beams, and presented the most appropriate methods and instruments for the young scientists' needs in the future. Participants were asked to pay particular attention to the complementary nature of X-ray and neutron techniques. The programme was made up of a common part followed by two parallel sessions: one for physicists and chemists, and the other devoted to the "structure and dynamics of biomolecules".

The programme of the school also included experiments on synchrotron radiation and neutron beamlines in either "hard matter" (neutron and X-ray powder and single crystal diffraction, EXAFS, imaging, inelastic scattering,...), in



"soft matter" (neutron and X-ray reflectivity, neutron and X-ray small-angle scattering,...) or in "biomolecular samples" (Multiwavelength anomalous diffraction, Laue diffraction, ...).

For the practicals' and tutorials' hands-on training, the students were divided into 17 experimental groups (4 students per group) and carried out experiments and data analysis set up by more than 100 local instructors. In this way, the students could establish contact with the scientists in charge at the large scale facilities, and therefore become familiar with the potential there. All full-time participants were assigned at least seven practicals and seven tutorials in the European Facilities, Grenoble Laboratories, LURE and Laboratoire Léon Brillouin. For practicals at LURE in Orsay and at Laboratoire Léon Brillouin in Saclay, students spent a few days in the Paris area.

The schedule was quite dense. However, there was time for the participants to enjoy some of Grenoble's sounds and Alpine sights. The school gave the students other opportunities for mingling with each other at the poster session, the skiing outing and the dinner party. Finally, the course ended with the now "classic" Wine-and-Cheese party offering a large palette of different wines and more than 40 different French cheeses!

HERCULES 2003

Higher European Research Course for Users of Large Experimental Systems

Grenoble,
2 March - 11 April 2003

Session A:

«Neutron and synchrotron radiation for physics and chemistry of condensed matter»

Session B:

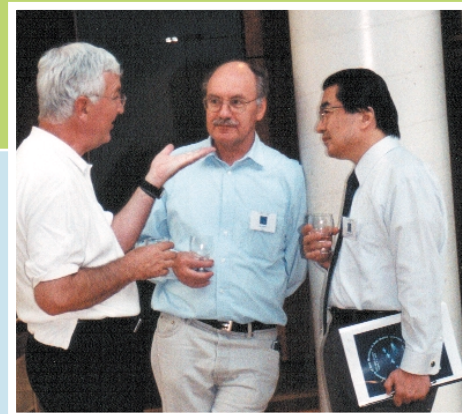
«Neutron and synchrotron radiation for biomolecular structure and dynamics»

Information:

Marie-Claude MOISSENET
Secrétariat HERCULES
CNRS - Maison des Magistères
BP 166 - 38042 Grenoble Cedex 9
Tel: 33 (0)4 76 88 79 86
Fax: 33 (0)4 76 88 79 81

e-mail:

marie-claude.moissenet@polycnrs-gre.fr
<http://www.polycnrs-gre.fr/hercules.html>



From left to right: Å. Kvick, A. Hewatt and Prof. Y. Fujii.

CRYSTAL CHEMISTRY

1 - 3 August 2002

The IUCr Satellite Meeting was held jointly by the ESRF and the ILL on 1-3 August 2002. The full title of the meeting was "Crystal Chemistry of New Materials and Soft Matter Studied by Synchrotron and Neutron Diffraction". The XIX Congress of the International Union of Crystallography was held in Geneva, Switzerland, on 6-15 August 2002.

Neutron and synchrotron diffraction have been essential for the understanding of new materials - hard magnets, superconductors, CMR (Colossal Magneto Resistance) materials, zeolites, etc. Large position-sensitive detectors, image plates, focusing optics, polarised beams and new software, are all being developed rapidly, and opening new

opportunities for chemists, physicists and biologists interested in relating the properties of materials to their structure. This workshop highlighted some of this new science, and the techniques that have made it possible. H. Schenk, the President of the International Union of Crystallography, stated "For young scientists, who were never before at big installations, the meeting in Geneva is an ideal opportunity to see the synchrotron and neutron facilities... in order to get a flavour of the opportunities they may provide for their future research." This satellite meeting should have provided the ideal opportunity for a new generation of scientists to explore the neutron and synchrotron radiation facilities available on the Grenoble site.

A total of 87 participants registered for the meeting, representing Australia, Denmark, France, India, Germany, Great Britain, Japan, the Netherlands and the United States.

It is our sincere hope that the satellite meeting sowed the seeds of multi-faceted scientific collaborations using the complementary methods of synchrotron and neutron diffraction.

Å Kvick and A. Hewatt

X-TOP

10-11 September 2002

The name of the X-TOP conference originates from a first X-ray TOPography-related meeting, held in Grenoble in 1990 and aimed at defining what was, at that time, the ESRF beamline devoted to diffraction topography. The X-TOP conference took place in Marseille 1992, Berlin 1994, Palermo 1996, Durham 1998 and Ustro-Jaszowiec 2000. These Conferences extended the topics well beyond 'topography' and incorporated other imaging and diffraction techniques (high resolution and grazing incidence diffraction, reflectometry, microtomography phase contrast imaging) which emerged or developed as a consequence of the availability of synchrotron radiation sources, in particular the ESRF.

170 participants coming from 21 countries attended X-TOP 2002. The first part of the Conference was held at the ESRF (10-11 September). It started with four 'basic' courses on 1) High Resolution Diffraction 2) Grazing Incidence Diffraction 3) X-ray Imaging techniques (Absorption, Phase Contrast, Bragg Diffraction) and 4) Standing

Waves. After visits to the various beamlines of interest for the participants (ID1, BM5, ID19, ID22 and ID32) the Conference moved (12 to 14 September) to the "Centre Paul Langevin", in Aussois. About 40 oral contributions (more than 80% used the "power-point - projector" possibilities) and more than 100 posters were presented there.

The conference covered a wide range of topics such as:

- New developments in methods and instrumentation (new imaging and diffraction methods mainly using synchrotron radiation, X-ray optics with special emphasis on the microfocusing and magnifying devices, data recording and processing, etc.)
- Applications to physical studies (defects, deformation, phase transitions, etc.)
- Characterisation of interesting materials (bulk crystals, layers and super-lattices, nanostructures, quantum dots, etc.)
- Theoretical aspects such as the predictions of dynamical theory when

using ultrashort pulses (new X-ray sources) or how valid are usual approximations of this theory when considering the new, layered or nanostructured, materials.

A number of e-mails were received at the ESRF, after X-TOP, thanking for what these participants considered to be a particularly interesting conference. This very rewarding aspect is surely the result of a conjunction of facts: firstly, of course, good science (the general scientific and presentation standard of these contributions was very high, and very lively discussions followed most of the oral talks or extended in front of the posters) but also a beautiful weather during the free afternoon, which allowed to enjoy the magnificent panoramas of the surrounding mountains, and a perfect, smooth, organisation. Last but not least, the general atmosphere of the meeting was very friendly, with a very successful "soirée dansante" and very good meals, the Aussois people even claiming that the X-TOP participants are the biggest cheese-consumers they ever had in their centre.

SELECTED SCIENTIFIC HIGHLIGHTS

X-ray Imaging Group

ID19 - Extension of "holotomography" to new scientific areas. (P. Cloetens, ESRF, and R. Mache, Génétique Moléculaire des Plantes-UMR 5575, Université Joseph Fourier, Grenoble)

Holotomography, which combines phase retrieval, using images recorded at several distances, and microtomography, is an elaborated phase contrast imaging technique developed at the ESRF. It has already been used successfully in metallurgical problems, such as the visualization of the phases in semi-solid alloys. It is now being extended to the Life Sciences (plants, vessels in the brain) and new materials (polymers and soft foams, carbon-carbon composites). New teams in the fields of Paleontology (fossil teeth) and the Earth Sciences are now using the imaging capabilities of the beamline.

ID21 - Zernike phase contrast X-ray microscopy at 4 keV photon energy with sub-100 nm spatial resolution. (U. Neuhäusler, ESRF, G. Schneider, Lawrence Berkeley National Laboratory, Berkeley, US, W. Ludwig, ESRF and INSA Lyon, Villeurbanne, France, M.A. Meyer and E. Zschech, AMD Saxony LLC & Co KG, Dresden, Germany and D. Hambach, Institut für Röntgenphysik, Universität Göttingen, Germany)

This article has been removed because of an error made in the production of the Newsletter. A corrected and extended version can be found in the ESRF Highlights 2002, pages 84-85.

New Group Structure

In order to facilitate communication and beamline operation, a new beamline group structure has been set up in the Experiments Division. The beamlines making up each group are listed in the Table.

The Group Heads and their deputies are appointed for three years with a possibility of renewal.

Beamline Reviews

The beamline reviews by panels of experts and normally chaired by SAC members are an essential part of the scientific development of the ESRF. They enable the management to propose future strategies and plans, and allow the general community to respond with corresponding ideas and comments. These reviews have brought considerable benefits to the ESRF and its scientific profile. Normally three beamlines from the 30 public and 10 CRG beamlines are reviewed every six months and at the time of the 44th SAC meeting the reviews will have covered all the beamlines in operation. It seems appropriate therefore to assess the overall review process. In most cases actions taken by the management of the ESRF following recommendations

Group (Group Heads)	Beamlines
Surface & Interface Science (S. Ferrer)	ID01, ID03, ID32
Soft Condensed Matter (G. Grübel)	ID02, ID10A, ID10B, ID13
X-ray Imaging (J. Baruchel)	ID17, ID19, ID21, ID18F, ID22
Macromolecular Crystallography (S. Mc Sweeney)	ID14A, ID14B, ID29, ID23
X-ray Absorption and Magnetic Scattering (N. Brookes)	ID08, ID12, ID20, ID24, BM29
High Resolution & Resonance Scattering (R. Rüffer)	ID16, ID18, ID22N, ID26, ID28
Materials Science (Å. Kvick)	ID09TR, ID09HP, ID11, ID15A, ID15B, ID30, ID31 (BM16)

made by the review panels have satisfied the requests and in many cases have opened up new scientific opportunities or techniques for the respective beamline. Three illustrative examples where Review Committee recommendations have produced significant developments are provided by ID2, BM16 and ID22.

- Beamline ID2 is now totally dedicated to soft-condensed matter studies and has been extensively modified to enhance the ultra-small-angle scattering (USAXS) capability and to extend the range of sample environment and use of detectors.

- The Powder Diffraction beamline, BM16, has now been transformed into an insertion device beamline ID31,

which should be ready for users later this year. BM16 itself will become a Spanish CRG, mainly dedicated to macromolecular crystallography. ID31 will be equipped with three 11-mm-gap undulators around a 10 mm vacuum vessel. The construction progress has been good and, at the time of writing, all the hutches and services are in place and a liquid nitrogen cooled monochromator is being commissioned and is performing above specifications.

- ID22/18F have been grouped together with ID21 under the leadership of a single scientist. This has led to a more efficient use of ESRF facilities and the development of micro-probe techniques with a concomitant expansion of the science programme.

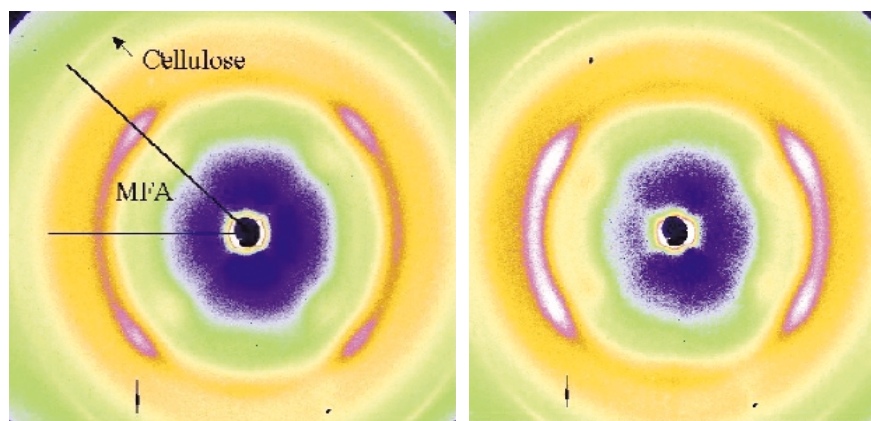


Fig. 3: The diffraction from wood fibres before stretching (left) and prior to failure (right). The symmetric peaks are due to the helical structure of the cellulose fibres and the position depends on the microfibril angle (MFA). As the sample is strained this helical structure is flattened causing a reduction in the MFA. In addition the weak outermost ring is due to diffraction from cellulose and moves to smaller Q with stretching.

Surface and Interface Science Group

ID1 - *In-situ* WAXS investigation of tensile stress and structure in wood slices. (J. Keckes and P. Fratzl, Montanuniversität Leoben, Austria, M. Hamilton, ESRF, M. Müller, Universität Kiel, Germany)

Wood represents a natural composite with the ability to adapt its structural properties to external mechanical requirements on all hierarchical levels. On the microscopic and nanoscopic scale, the structural optimisation of the mechanical behaviour of wood is closely related to the cell wall microstructure and, especially, to the magnitude of the microfibril angle (MFA). The aim of these studies was to characterise microstructural changes in wood slices under external loading using wide-angle X-ray scattering. Wood foils of dimensions 5 x 50 x 0.2 mm were strained in a tensile stage under various strain rates monitoring stress response and collecting X-ray diffraction patterns (XRD) using a 2-D CCD detector.

By relating stress-strain curves and XRD results, it was possible to evaluate changes of MFA, MFA distribution and microscopic strain as a function of external strain and strain rate in the slices (see **Figure 3**). The results document an elastic response of the wood microstructural parameters that depends sensitively on the magnitude of external strain and differs significantly for different types of wood. However, the strain rate was not found to play an important role. The *ex-situ* XRD investigations of the wood slices do not indicate any significant remaining changes of MFA in comparison with the original value.

The comparison of the mechanical and the micro-structural results from three different compression wood types

allows general conclusions to be drawn regarding the roles of different microstructural features of wood on the mechanical behaviour. It also shows how wood architecture units are progressively optimised during evolution.

Macromolecular Crystallography Group

ID14 - *The interaction of antibiotics with ribosomes* (F. Schlünzen¹, R. Zarivach², J. Harms¹, A. Bashan², A. Tocilj³, R. Albrecht³, A. Yonath², F. Franceschi³ with affiliations:

1. Max Planck Research Unit for Ribosomal Structure, Hamburg, Germany.
2. Department of Structural Biology, Weizmann Institute, Israel.
3. Max Planck Institut für Molekulare Genetik, Berlin, Germany).

Bacterial ribosomes are the targets for many antibiotics that prevent the production of new proteins in cells, thus killing the bacterium that is targeted. The recent elucidation of the three-dimensional structures of a number of ribosomal subunits has opened the way for a detailed visualisation of ribosome-antibiotic interactions. Using single crystal X-ray diffraction data recorded at ID14, the crystal structures of a number of clinically important antibiotics have been obtained in complex with the large 50S ribosomal subunit of the extremophile bacterium *Deinococcus radiodurans* (**Figure 4**). These show that the antibiotics studied bind only to the ribosomal RNA. They

function either by inhibiting the actual synthesis of new proteins or, as is the case for the macrolide class of drugs, by blocking the channel through which the newly synthesised protein is channelled away from the site of the peptide bond formation. The structures show in atomic detail how the antibiotics function and, perhaps equally importantly, how known mutations in the nucleotide sequence of the ribosomal RNA have led to resistance against the antibiotics studied. The studies also suggest approaches that may enable the rational design of new, therapeutically relevant antibiotic drugs in the future.



Fig. 4: The structure of the large ribosomal subunit from *D. radiodurans* (green) in complex with the macrolide erythromycin (red). Note that, upon binding to the ribosome, the antibiotic partially blocks the exit channel for the nascent peptide.

X-ray Absorption and Magnetic Scattering Group

ID8 - Magnetic speckle

(Collaboration between J.F. Peters, M.A. de Vries, O. Toulemonde, J. Miguel, J.B. Goedkoop, Van der Waals-Zeeman Institute, Amsterdam, The Netherlands, and S. S. Dhesi and N. B. Brookes, ESRF)

Nano-scale structures are best seen with nanometre wavelengths, such as found in the soft X-ray range. In this energy range are also found the strongest magneto-optically active core-valence resonances, making soft X-rays a powerful tool for the study of nano-magnetism.

The coherent radiation that can be obtained at the ESRF has been used in a series of magnetic speckle experiments. In **Figure 5** a coherent beam has been used, as evidenced by the Fraunhofer fringes of the transmitted beam (central image). As a result, the first order maxima fragment into a clearly defined speckle pattern, with strong intensity contrast and clear inversion symmetry (left and right images).

Such speckle patterns reflect the exact structure of the illuminated area, and fluctuations in the magnetic structure result in fluctuations in the speckle intensity. This is exploited in dynamical X-ray scattering, so far only used in studies of colloidal particles to address the dynamics of the system at time scales of microseconds to seconds. The magnetic speckle patterns show that it should be possible to do the magnetic equivalent of this technique, which would be extremely useful for the study of the thermodynamical behaviour of magnetic ordering in bulk, surfaces and small particles.

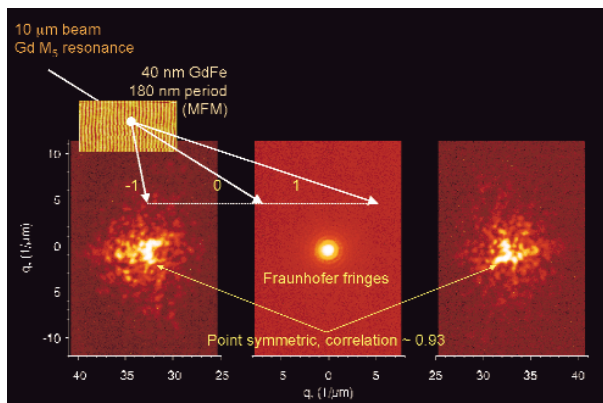


Fig. 5: Coherent first-order magnetic diffraction peaks from aligned magnetic stripe domains: Magnetic X-ray speckle.

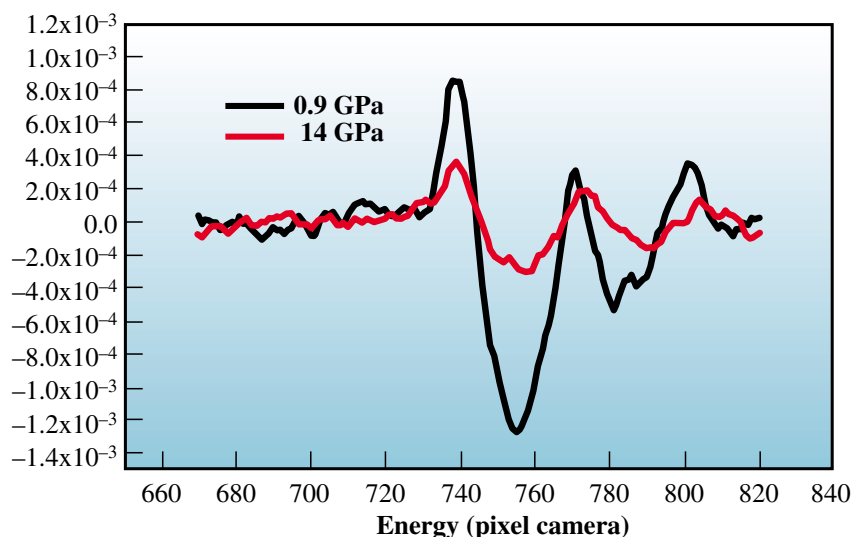


Fig. 6: Fe₃Pt: XMCD under pressure at the Fe K-edge.

ID24 - High pressure X-ray magnetic circular dichroism at the Fe K-edge

(O. Mathon¹, F. Baudelet², J.P. Itié³, A. Polian³, and S. Pascarelli¹
1. ESRF, Grenoble, France. 2. Physique des Milieux Condensés, Univ. Pierre et Marie Curie, Paris, France. 3. LURE, Centre Universitaire Paris Sud, Orsay, France)

XMCD experiments provide an element-specific mapping of s-, p- or d-electron spin and orbital densities in solids using the magnetic absorption characteristics of circularly polarised synchrotron radiation. The development of dedicated beamlines producing a high flux of circularly polarised synchrotron radiation using, like on ID24, the elegant technique of a quarter-wave phase plate, enables new applications of XMCD spectroscopy such as high pressure studies. XMCD of 3d transition metals under pressure has long been a forbidden field, due to the impossibility of accessing the L-edges of these elements because of the highly absorbing properties of high pressure cells in the soft X-ray range. On the other hand, the XMCD signal at the K-edges is about 2 orders of magnitude smaller, and all attempts to measure these signals through diamond anvil cells had failed up to now. Very recently such measurements have finally become possible on beamline

ID24 (see **Figure 6**). The first applications are related to the simultaneous XAS and XMCD study of the Fe bcc-hcp phase transition at around 15 GPa, and to the understanding of spin hybridisation as a function of inter-atomic distances in 3d-5d INVAR alloys.

Materials Science Group

ID15A - In-situ studies of oxidation at a solid-liquid interface

(H. Reichert, M. Denk, I. Ramsteiner, C. Mocuta and A. Schoeps, MPI für Metallforschung, Stuttgart, Germany)

Technically important processes for real materials often involve interfaces between solid and liquid components. Such interfaces are usually covered by intervening oxide layers.

Reactions at such interfaces are intrinsically difficult to investigate for *in situ* experiments. Reflectivity studies, **Figure 7(a)**, were carried out employing the high energy X-ray microbeam at beamline ID15A. In the experiments the time evolution of the structure of a deeply buried lead oxide layer normal to the interface between liquid lead and solid silicon was investigated. Careful data analysis of the electron density profile, **Figure 7(b)**, across the solid-liquid interface provides evidence for a slow transfer of the oxygen atoms from the lead oxide layer to the silicon, thereby indicating internal oxidation of the silicon.

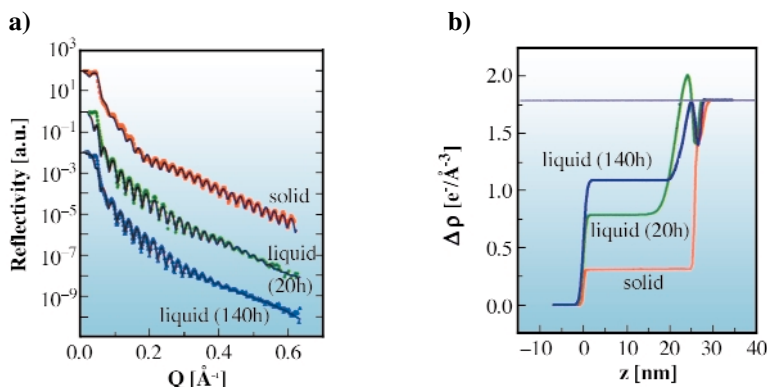


Fig. 7: (a) Reflectivity curves of a solid Pb – solid Si interface with a liquid Pb – solid Si interface after 20 hours and 140 hours. (b) Electron density profiles across the Pb – Si interface.

ID30 - Breakdown of intermediate-range order in liquid GeSe_2 at high pressure (W.A. Crichton, M. Mezouar, T. Grande, S. Stolen and A. Grzechnik, *Nature*, 414, 622-625 (2001))

Studies of liquids with tetrahedral coordination, particularly during compression or quenching, have indicated the existence of distinct phases in the liquid state, distinguishable by density and local structure. In systems that exhibit critical phenomena in the super-cooled state, anomalous behaviour of the compressibility is also anticipated above the critical point, as revealed by simulations of water. Liquid GeSe_2 is a potentially attractive system for studying both types of phenomena, given its two-dimensional tetrahedral structure and anomalous physical properties (including a density maximum near its melting point). *In situ* X-ray diffraction measurements have been performed at the high pressure beamline ID30 revealing that the structure of the liquid is sensitive to pressure and that anomalous compressibility is expected. During compression of liquid GeSe_2 , the connectivity of the liquid changes from two- to three-dimensional, leading to a breakdown of the intermediate-range order. The gradual change in structure above the melting line may develop to a first-order liquid-liquid transition in the super-cooled regime.

High-Resolution and Resonance Scattering Group

ID16 - Evidence of a spectroscopic Kondo scale in ytterbium compounds (C. Dallera, Politecnico di Milano, Milano, Italy; M. Gironi, Ecole Polytechnique Fédérale, Lausanne,

Switzerland; A. Shukla and G. Vankò, ESRF, Grenoble, France; J.L. Sarrao, Los Alamos National Laboratory, Los Alamos, USA; J.P. Rueff, Université P. et M. Curie, Paris, France; D.L. Cox, University of California, Davis, USA)

Bulk-sensitive resonant inelastic X-ray scattering (RIXS) measurements performed at ID16 reveal with unprecedented clarity the existence of characteristic Kondo scales in heavy fermions. In YbInCu_4 and YbAgCu_4 RIXS selectively probes the Yb^{2+} component of the hybrid ground state and directly yields the temperature dependence of the Yb 4f occupation. A sudden valence change at a phase transition in YbInCu_4 but a continuous temperature dependence in YbAgCu_4 are observed, consistent with the predictions of the Anderson Impurity Model, for a Kondo temperature $T_K = 70$ K. These results solve a long-standing controversy on the applicability of the Anderson model to spectroscopic properties, and establish RIXS as a quantitative probe of the electronic structure of strongly correlated electron systems.

ID18/ID22N - Size and oxidation effects on the vibrational properties of nanocrystalline α -Fe (L. Pasquini, A. Barla, A. I. Chumakov, O. Leupold, R. Rüffer, A. Deriu, E. Bonetti, University of Bologna, University of Parma, I.N.F.M., ESRF)

Nanostructures and nanocrystalline materials gain more and more attention in various fields both in applications and fundamental research. Recently, "Magnetic order in ultra small iron islands on tungsten (110)" was reported (ESRF Highlights 2001 p.69). However, not only the magnetic properties are

crucial for the fabrication and functioning of nanostructured devices, but also their dynamic behaviour. The investigation of vibrational dynamics is of primary importance for the understanding of properties like thermal expansion, heat capacity, thermal conductivity, and vibrational entropy. The vibrational density of states (DOS) plays a key role in this respect. In order to determine the DOS of nanocrystalline α -Fe, the recently developed technique of nuclear inelastic scattering (NIS) of synchrotron radiation was employed. Various samples were prepared by inert gas condensation with different crystallite size in the 6-13 nm range and at different oxidation levels. The measurements showed an enhanced population of low-energy vibrational modes, which arises from the high fraction of interfacial sites, connected with the small crystallite size. Oxidation similarly contributes to the low-energy DOS but additionally brings about stiff modes above the high frequency cut-off of bulk α -Fe. Broadening of the DOS peaks due to reduced phonon lifetime in the nanometre-sized crystallites is observed. All measured samples exhibit a Debye-like behaviour with the low-energy tail of the DOS essentially quadratic in energy.

These findings are quite surprising. Due to the confined geometry a remarkable change in the dynamical behaviour would have been expected, especially in the low-energy regime. This was also indicated by other investigations.

Soft-Condensed Matter Group

ID2 - Mechanism of cancer invasion in human breast tissue (P. Suortti et al., University of Helsinki and V. Urban, ESRF)

A comprehensive study of the supra-molecular structural features in human breast tissue samples containing healthy and cancerous regions, using small-angle X-ray scattering (SAXS), has been conducted. Most importantly, all SAXS patterns in this study have been correlated with the histo-pathological classification of the tissue at a spatial resolution of 250 micrometers. It has been reported recently that scattering patterns far from tumours are different from those of tumours. The present study, however, gives a much more detailed picture of the local structural changes and underlying biochemical processes, when cancer invades healthy tissue. A model has been

developed that allows quantitative interpretation of the scattering patterns in terms of the amounts of different types of tissue (adipose/connective, healthy/invaded/necrotic) that are present in a scattering volume of 0.04 mm³. The results provide new insights into the mechanism of cancer invasion of healthy tissue. In addition, they are invaluable in that they demonstrate the possibilities and limitations for new scattering based methods of mammography.

ID10B - Nucleation and growth of inorganic crystals of polymer monolayers at the air/solution interface. (A. Berman, Y. Golan, Y. Lifshitz Ben-Gurion University, Beer-Sheva, Israel and O. Konovalov, ESRF)

Long chain amphiphilic compounds have been shown to nucleate inorganic and organic crystals at specific faces, with matching interfacial structure and chemistries. A polydiacetylene (PDA) film was used to nucleate CdS crystallites in an ordered manner. Monolayer films were prepared on a Langmuir trough by spreading the monomer compound (10,12 pentacosadiynoic acid) on a water sub-phase from chloroform solution, followed by compression to the required surface pressure and UV polymerisation. This results in a film with remarkable structure

that is characterised by parallel strands of the linear conjugated polymer. The sub-phase is then replaced by peristaltic pump with 0.5mM CdCl₂ solution. The addition of Cd²⁺ ions to the acidic films head groups causes the films to reorganize in a more compact manner due to formation of salt bridges between neighbouring strands. Crystallisation is induced by infusion of small amounts (ca. 250-500 µl) H₂S into the trough chamber. The grazing incidence diffraction technique was applied to study the system at various stages of the experiment; (a) PDA film on water; (b) PDA film after photopolymerisation induced with UV; (c) PDA film on cadmium solution; (d, e) during and after CdS crystallisation. Structural parameters of the film at different pressures and characteristics of *in situ* nucleation and growth of inorganic crystals (size, orientation and in-plane organisation) have been obtained.

Industrial Beamline

ID27 - Mapping the contamination distribution on semiconductor wafer surfaces

(R. Barrett, E. Papillon, M. Navizet, S. Arnoux, R. Hino, ESRF)

The control of surface contamination

levels is critical for current and future semiconductor manufacturing processes. Consequently advanced metrology techniques are necessary to provide appropriate monitoring of contaminating species. TXRF is a commonly used technique to provide the necessary quantitative elemental surface concentration data. Unfortunately the commercially available machines based upon rotating anode sources are reaching their limits in terms of the detection sensitivity. One way of improving detection limits is to chemically concentrate the contaminant species from the whole wafer surface into a droplet and to analyse the resulting concentrated drop or its dried residue by classical analytical techniques or TXRF. This method sacrifices important information regarding the spatial distribution of contaminant species that may be of use in determining the source of the contamination. The ID27 Total Reflection X-ray Fluorescence (TXRF) beamline circumvents the need for pre-concentration by offering at least 20 times of improvement in the detection sensitivity (~ 3·10⁸ atoms/cm² for Ni) for individual measurements over conventional TXRF. Moreover, by using a multi-element detector to fully exploit the available flux from an undulator source it is possible to map simultaneously the contamination from 6 (12) points on the 200 (300) mm wafer. This unprecedented combination of an improvement in detection sensitivity and increased number of measurement points allows high sensitivity mapping of the wafer contamination distribution. **Figure 8** shows respectively the a) Fe, b) Cu and c) Zn distribution over a 200 mm silicon wafer.

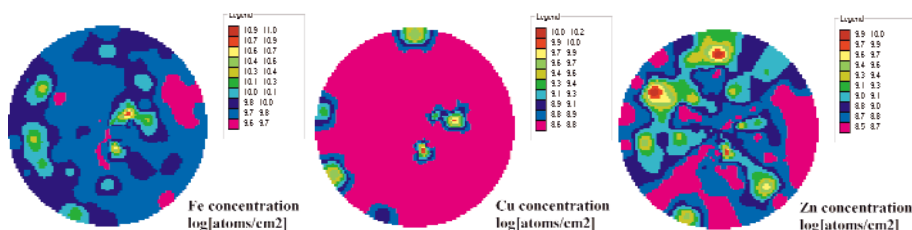


Fig. 8: Spatial distribution of metallic surface contamination on a 200 mm diameter silicon wafer substrate. The surface concentrations are displayed on a log scale.

POLYMER WORKSHOP FOR INDUSTRY

8 February 2002

A dedicated workshop was held on Friday 8 February at the ESRF specifically aimed at polymer producers and transformers. The aim of this meeting was to give the participants an opportunity to discover the facilities of the ESRF as well as the various possibilities that the ESRF can offer in this field. A total of 14 participants took part, from major companies such as Becton Dickinson, AtoFina, Honeywell and Rhodia, as well as a number

of smaller companies. Most of the participants came from France, but 4 also made the trip from Italy and Germany. After a presentation of the ESRF made by W.G. Stirling, short talks were given by C. Riekkel, T. Narayanan, W. Bras and J. Baruchel on different applications of synchrotron radiation to polymers. J. Doucet then explained the various access modes available to industry. After lunch, the participants were given a guided tour of the facilities and several

beamlines, some of which already work with industry. The participants showed a real interest and promising contacts were established.



NEWS FROM THE CRGs

On the **BM30** port a new French beamline (**FAME**) was installed that opened to regular users in July 2002. Its main objective is the application of X-ray Absorption Spectroscopy to the structural investigation of very dilute systems in Environmental, Material and Biological Science. FAME will be able to focus the beam down to $3 \times 3 \mu\text{m}^2$ using a Kirkpatrick-Baez mirror system [1]. **Figure 1** shows the first absorption spectrum of a diluted sample containing 40 ppm chromium obtained on this beamline.

BM14/BM16: By the end of this year the former ESRF beamlines BM14 and BM16 will become CRG beamlines. BM14 will be sold to a UK group (MRC, BBSC, EPSRC [2]), while BM16 will be converted into a Macromolecular Crystallography beamline with full MAD capability and sold to the Spanish Ministry of Science and Technology, which will add at its own expenses an additional station to carry out small-angle scattering and diffraction experiments. This conversion process is fully underway and the start of the commissioning phase is foreseen for January 2003.

The team of BM14 have recently been successful partners in obtaining funds from the BBSRC e-science program to develop an easy-to-use resource for protein crystallographic structure determination [3]. The aim is to unify the procedures of protein structure determination into a single all encompassing interface from which users can initiate, plan, direct and document their experiment either locally or remotely from a desktop computer.

Scientifically, Joan Aymami, Miquel Coll (IBMB Barcelona) together with the BM14 and ID14 teams contributed to investigations of Cryotolepin, a traditional cure for malaria in Africa. This substance may as well have a therapeutic potential in treating cancer due to its role in inhibiting DNA replication and transcription. The researchers solved the structure of Cryotolepin and demonstrated the mechanism of its insertion into the DNA strand [4]. Studies in drug design will follow.

The Spanish CRG beamline **BM25 (SpLine)** got its two monochromators delivered. Their installation and subsequent commissioning have been started. Both double-crystal monochromators, designed by the Spanish team, use a novel sagittal bender for the second monochromator crystal which is equipped

with a unique central pneumatic bender. With this delivery, SPLINEs final construction phase is reached. It is expected that the commissioning phase will be started during the second half of 2003.

The second UK CRG beamline, **BM28 (XMAS)**, spread good news in July 2002: This beamline got a new 5 year grant funding it until 2007, the funds allowing to hire a third beamline scientist! Following suggestions of the last ESRF review of XMAS, a closer cooperation between XMAS, the staff of the ESRF beamline for magnetic scattering (ID20) and the ESRF theory group is aimed at. To exchange views, plans and perspectives, a successful workshop was organized on September 13 bringing together these groups and potential users. XMAS/ID20 is a very good example of the benefits for the user community arising from closer cooperation between ESRF and CRG beamlines.

Conventional solid state X-ray detectors show an energy resolution of about 100-200 eV within the regime of hard X-rays. Cryogenic detectors (microcalorimeters) based on Transition Edge Sensors are a promising alternative, the small thermal fluctuations of which can in principle lead to energy resolutions of several eV. This type of detectors is

used for example for the measurement of high-resolution beta-decay spectra in Neutrino Physics [5]. For the first time the team of the Italian CRG beamline, **BM8 (GILDA)**, tested such a device on a synchrotron beamline using a $300 \times 400 \mu\text{m}^2$ Sn absorber of 25 μm thickness (adapted to a good efficiency at 10 keV) attached to a TES sensor (Al/Ag multilayer biased across the superconductivity/normal transition which is 500 μK wide). The temperature pulses generated within the Sn absorber by the incoming photons are converted into a current signal by the TES sensor. **Figure 2** shows the X-ray L fluorescence spectrum of Re measured using this device in a preliminary test experiment leading to an energy resolution of 70 eV.

References

- [1] <http://www.esrf.fr/exp-facilities/BM30B/BM30Bb-en.html>
- [2] <http://www.bm14.ac.uk>
- [3] <http://www.research-councils.ac.uk/escience>
- [4] Lisgarten, J.N., Coll, M., Portugal, J. Wright, C.W. Aymami, J. Nature Structural Biology **9**, 57 (2002)
- [5] F. Gatti, F. Fontanelli, M. Galeazzi, A. M. Swift, S. Vitale, Nature **397**, 137 (1999)

Fig. 1: Absorption spectrum of a diluted sample containing 40 ppm chromium.

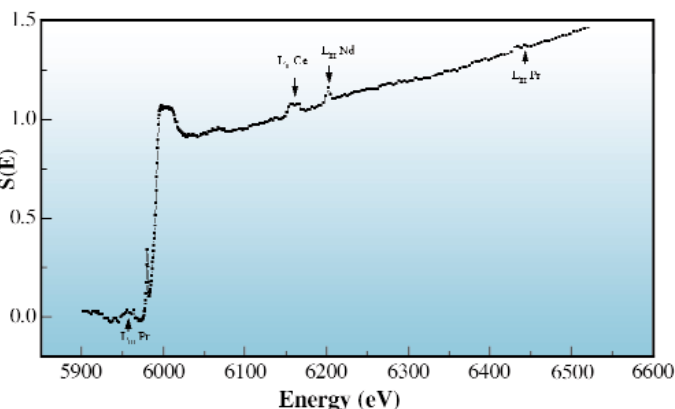
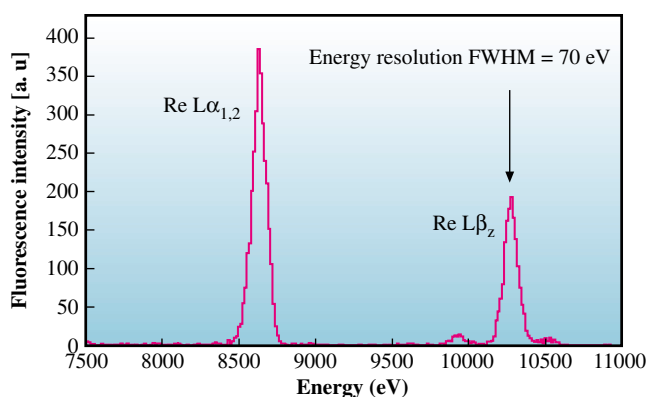


Fig. 2: X-ray L fluorescence spectrum of Re.





J.M. Gibson (APS Director – on the right) with K. Harkay from the APS Machine Group.



W.G. Stirling in discussion with A. Kira (Spring-8 Director).

THREE-WAY MEETING

14-15 November 2001

On Wednesday 14 and Thursday 15 November the ESRF hosted the APS – ESRF – Spring-8 meeting, which is held about every 18 months. The programme had been designed to cover as much as possible overlapping fields of interest indicated beforehand by the three facilities. Thus groups of some ten accelerator or beamline instrumentation specialists from each of the three labs had an intense exchange of experiences and discussed future projects in fields such as beam stability, insertion devices, top-up mode, increase of beam current, X-ray optics (a three-way optics workshop had preceded the meeting), beamline automation, detectors and developments for next generation sources. One session was dedicated to managerial issues such as access to beam time, information strategies, funding and audit. The Directors of APS and Spring-8, J.M. Gibson and A. Kira, both of whom had been appointed only shortly before the meeting, appreciated this dense but nevertheless rather informal way of communication. In the summary session, prospects for collaborative projects were discussed as well as concrete means of how to foster them in the interest of all three facilities.

X-RAY OPTICS WORKSHOP

12-13 November 2001

A workshop on “X-ray Optics” was held at the ESRF on Monday 12 and Tuesday 13 November as a satellite event to the APS-ESRF-Spring-8 Three-Way Meeting. The aims of this first three-way workshop organised at the ESRF by A. Freund with the efficient help of L. Stride were to bring together the optics specialists of the three facilities, to discuss matters of common interest and concern, to exchange information and experience and to identify subjects for collaborative projects. We were pleased to receive 10 experts (7 from the APS and 3 from Spring-8) and about 20 participants from the ESRF attended the workshop. The meeting started with overviews of activities conducted and recent results obtained at the APS, Spring-8 and the ESRF. They were followed by presentations

on particular issues such as the state-of-the-art surface and interface quality and on the performance of mirrors and multilayers, respectively, the quality of beryllium windows, microfocusing by Kirkpatrick-Baez systems, ultrahigh resolution monochromators, the quality of presently available diamond crystals, laboratory and beamline-based metrology and characterisation facilities, the limits of cryogenic cooling and computer simulations to model and predict the performance of one or several combined optical elements on synchrotron beamlines. Much time was provided for discussions and particular emphasis was put on laboratory visits and exchange of experience, multilayer deposition

and characterisation and tests on the beamline BM5. It was also felt that the three-way meeting was a good occasion to meet and discuss the present and future, and that therefore the next workshop should be held at the APS in about 18 months. In the meantime we will continue to enhance collaboration by mutual exchange of information and experience including staff exchange and by performing common studies and experiments at the three facilities.





FAME38 AT ILL/ESRF

FaME38 is a new Facility for Materials Engineering that has been set up jointly by ILL/ESRF. Its aim is to provide the extra support required to enable European engineers to make the best use of neutron and X-ray beam facilities. The 40-month start-up phase of the project is funded by an EPSRC grant of Euro 2.5M that is administered through the University of Salford on behalf of seven collaborating research institutions. Matching on-site support is provided by ILL/ESRF. The team of A. Dale (administrator), Drs. D. Hughes and H. Sitepu (research fellows) and B. Malard (technician) began work on-site in April 2002. The project manager is Professor P. Webster who spends half of each month with the project. The unit is physically located at the ILL but will provide services equally to all academic and industrial engineering users of both ILL and ESRF.

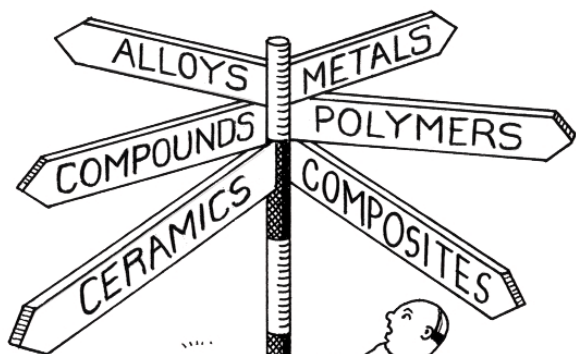
The basic philosophy of FaME38 is that ILL and ESRF are very well

equipped to support the broad range of science for which they were founded but have not been similarly resourced to provide the extra and specialised support that is required by engineers to perform engineering research. Until now most 'engineering' research at the facilities has been done by applied scientists, rather than by engineers. Typically they have found that the equipment and software available was not optimised for engineering measurements, particularly for users with limited scientific background. For example a substantial proportion of allocated beam time has been wasted positioning complex-shaped components on-line in preparation for strain scanning. The principal objective of FaME38 is to deliver, in close collaboration with beamline staff, the extra facilities and support that engineers need.

FaME38 will provide engineering users with a "Technical Centre" equipped with a co-ordinate measuring machine to

determine complex and distorted component shapes, together with facilities to simulate and optimise scans off-line before starting measurements on-line. Its materials laboratory will have micro-structural characterisation and static and dynamic thermo-mechanical loading equipment. Its "Knowledge and Training Centre" will provide technical and scientific know-how. Users will be helped to draft proposals, to plan and prepare experiments off-line, and be assisted with data collection, on-line processing and analysis. FaME38 will provide a focus and user facility for European engineers wishing to make use of Central Facilities. Its focus is on developing strain imaging facilities at ILL/ESRF but is likely also to stimulate and support the engineering use of SANS, SAXS, radiography and tomography. All academic and industrial engineers with interests in diffraction techniques are invited to contact FaME38 at FaME38@ill.fr.

Your choice



Metals, Alloys,
Ceramics, Polymers...

If you're looking for small quantities of any of these, then look no further...

Our range of materials is second to none and includes foils, rods, wires, tubes and many other forms. And in case you can't find precisely what you need, then our custom manufacturing service may be just what you're looking for.

So put an end to fruitless searches - contact Goodfellow!

Goodfellow

Goodfellow Cambridge Limited

Ermine Business Park, Huntingdon, PE29 6WR, Great Britain

Tel: 0800 731 4653 or +44 (0)1480 424 800

Fax: 0800 328 7689 or +44 (0)1480 424 900

E-mail: info@goodfellow.com Web: www.goodfellow.com

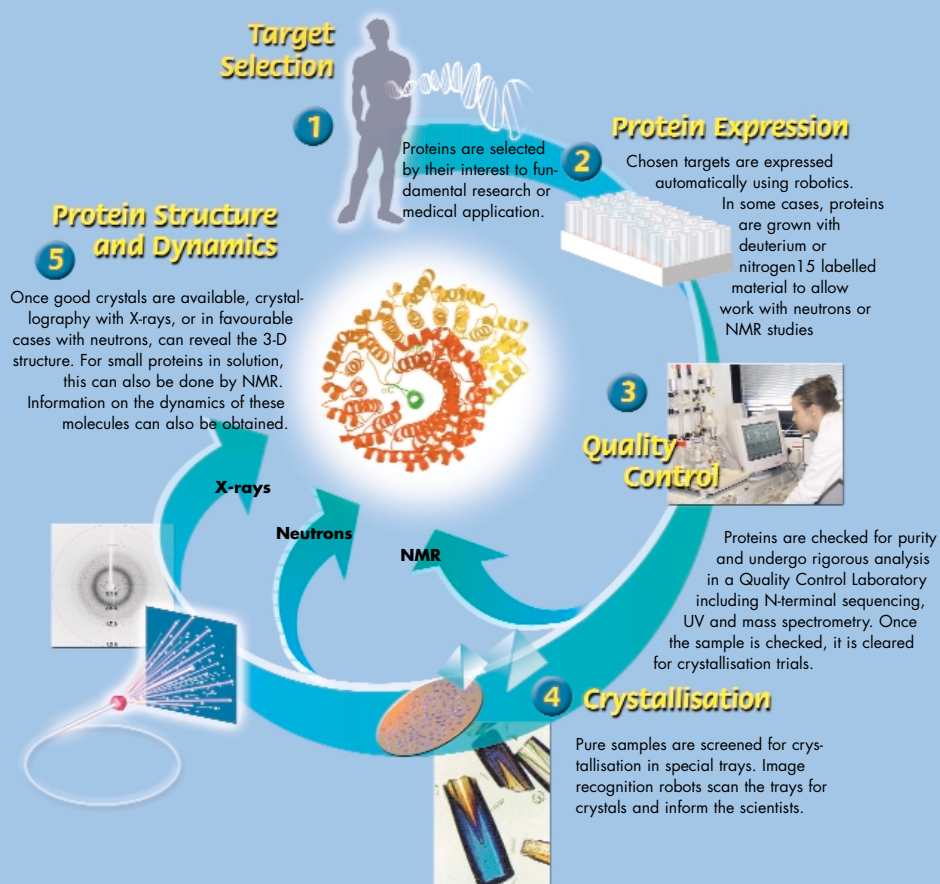
THE PARTNERSHIP FOR STRUCTURAL BIOLOGY: A EUROPEAN CENTRE OF EXCELLENCE

The ESRF, the Grenoble Outstation of the EMBL, the ILL and the IBS are joining their forces to form the Partnership for Structural Biology (PSB). This coalition will bring together the many different yet essential skills and resources needed to pursue an integrated European Programme in Structural Biology. The programme will involve the construction of a new state-of-the-art beamline at the ESRF and the construction of purpose-built laboratories in a new building on the ESRF/ILL/EMBL site.

The Post-Genomic Era: 21st Century Structural Biology and Medicine

Today's research in biology concentrates on a better understanding and treatment of human diseases. The Human Genome Project has already produced an enormous body of information about the sequences of the human genome (specifying up to 100,000 proteins), which is believed to represent the foundations for a clear picture of how the human body functions at the molecular level. The science of proteomics looks at the interactions between proteins that make our bodies work. These interactions change dynamically with the protein expression in any one cell varying dramatically as genes are turned on and off in response to environmental changes (for example cold, radiation damage, or disease causing mutations). Information on the structure, function and interaction of these tens of thousands of proteins is required in order to exploit the new panoply of data for revolutionary human disease treatments.

However, at present, knowledge of the structure of most of these proteins is lacking and their detailed three-dimensional structures will need to be determined if the structure-function relationships are to be understood and used medically. Recent advances, advances that are still continuing apace, in every step of protein structure determination from target selection to protein expression and crystallisation to data collection, processing and phasing, now allow structures to be determined rapidly. It is clear that X-ray crystallography will play a leading role in structural studies and the use of high-throughput macromolecular



crystallography facilities at synchrotron radiation sources will be essential to build the database of three-dimensional protein structures. Nuclear Magnetic Resonance techniques and, for certain problems, neutron scattering constitute further important tools for this type of studies contributing information complementary to X-ray crystallography.

A Unique European Centre of Excellence

This coalition of four major research institutes to form the PSB,

located close together in Grenoble, and the pool of resources that they together provide, is targeted to support and strengthen the various national and European Union initiatives now underway in Europe and enable the formation of a European structural biology centre on the Grenoble site. The aim is that the PSB should play an important role in European structural genomics programmes focussed on proteins of medical interest, capable of taking part in the scientific as well as technical development and training aspects of such a programme.

A Blueprint for Success

1. State-of-the-Art Beamline

As part of the PSB, the ESRF will expand its macromolecular crystallography capacity with a new highly-automated dual station public beamline, ID23. The line will make use of a canted undulator system on the ESRF storage ring that will produce two X-ray beams diverging by 1.5 mrad and thus permit two beamlines to operate with minimal interference. One of these will have a fully energy-tuneable (7-20 keV) Multiple-wavelength Anomalous Dispersion (MAD) station and the other a fixed-energy station (see **Figure 1**). By fixing the energy of the side station most of the components of the existing macromolecular crystallography beamlines can be adapted to the new lines thereby considerably shortening construction lead time. At the foreseen energy of 14.0 keV anomalous dispersion data can be collected from all the most commonly used elements in macromolecular crystallography permitting the station to serve a wide range of experiments including de novo structure determination.

The first phase tunable station is due to be operational from autumn 2003 and the second station around twelve months later.

2. Dedicated Laboratories

The Members of the Partnership will use their resources to construct and equip a new building to act as a focus for structural biology on the site. For the first phase, the size of this building has been fixed to about 1,400 m² of useable surface area, at an estimated cost of 3.6 M (excluding costs for experimental equipment). It will house the activities of the Partnership, including:

- offices and laboratories for the activities of the ESRF/EMBL joint structural biology group (JSBG)
- offices and laboratories related to the ESRF's structural biology programme
- the expanded activities of the ILL biology group including the ILL/IBS/EMBL biomolecule labelling facility
- EMBL infrastructure for high throughput protein expression, characterisation and crystallisation
- a Quality Control Laboratory operated by the IBS
- infrastructure for data analysis.

In a second phase, the building shall be expanded in order to provide offices and laboratories that can be let to external groups, companies or consortia working in the field of structural biology.

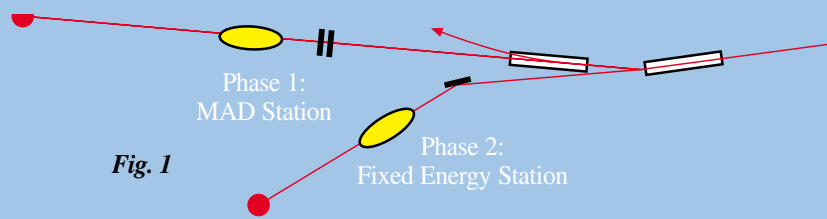


Fig. 1

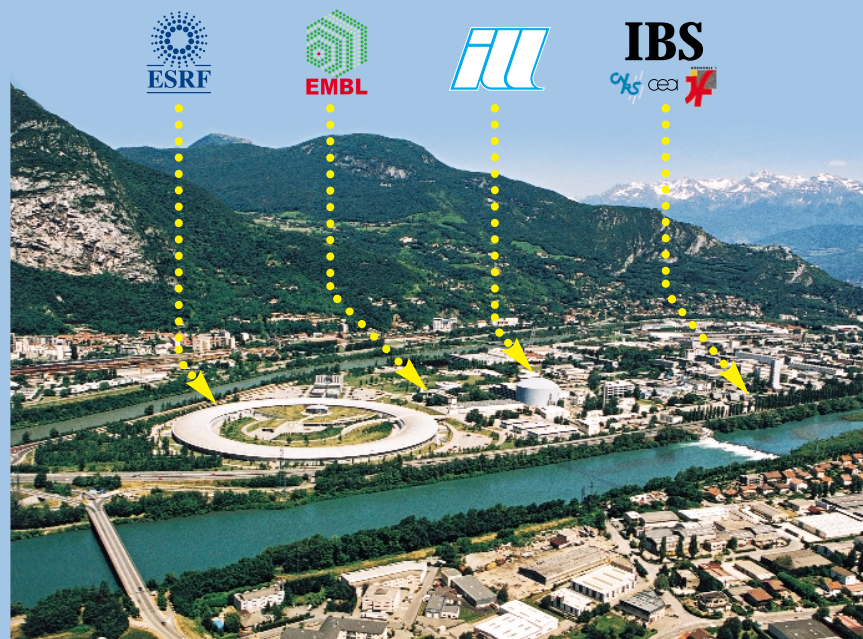
ASSOCIATE PSB MEMBERS

Aside from the four Partners, it is essential to involve industrial concerns and other interested parties in the PSB activities. Individual companies, both established pharmaceutical enterprises and promising start-up firms, are being invited to become Associate Members of the PSB. Such membership will involve a membership fee and an annual subscription and will guarantee access to a certain number of shifts at the ESRF macromolecular crystallography beamlines for a period of three years, at the current rates for the sale of beam time. In this way it is thought that the PSB will attract sufficient external income to fulfill its basic plans as well as creating a site for cross-academic and industrial collaborations.

The PSB combines the skills and resources of four leading institutes, sharing a common goal and enabling

a fully interdisciplinary approach involving biologists, crystallographers, chemists, engineers, computer specialists and experienced managers. It is clear that such an initiative will be essential if other European Union and national programmes are to function in the most effective manner. Collaborations with these other programmes will be established as they are funded and commence research.

It is essential that a strong relationship is created between the PSB (and its component institutes) and appropriate industrial concerns. Whatever the form and depth of intra-industry collaboration, it is crucial that the PSB is seen as a willing and effective collaborator. Of course it is also these commercial concerns that will be the means of delivering the fruits of the hoped for medical revolution to humanity.



ESRF • European Synchrotron Radiation Facility

Europe's brightest synchrotron radiation source

Has a major programme in structural biology which will be strengthened by a new world-class crystallography beamline.

EMBL • European Molecular Biology Laboratory

EMBL Grenoble Outstation with strong expertise in molecular structural biology.

Will build a core infrastructure for high-throughput protein expression, characterisation and crystallisation.

ILL • Institut Louis Langevin

The world's leading neutron source

Is building, in collaboration with EMBL and IBS, a laboratory for deuteration/labelling of biological macromolecules to exploit the full power of neutron scattering methods.

IBS • Institut de Biologie Structurale

One of France's premier structural biology institutes

Will bring a unique platform including NMR, mass spectrometry, cryo-electron microscopy and analytical ultracentrifugation.

FUTURE X-RAY FACILITIES

P. Elleaume, Machine Director

In the past few years, intense activity has been deployed worldwide to identify the most promising concepts for future large-scale X-ray facilities. Three schemes have been identified. They are the conventional storage ring type facilities, the linear accelerator based sources making either use of the Self Amplified Spontaneous Emission (SASE) version of the Free Electron Laser (FEL) or the energy recovery. The purpose of this article is to present the status of progress in the development of these sources.

Storage Ring Based Sources

The storage ring based synchrotron light source has been one of the most important success stories of accelerator technology in the past 30 years. In the 1960s early storage rings were designed as electron-positron colliders to be used for particle physics. The merit of synchrotron radiation was very quickly recognized and, in the 1970s, it started to be used in many laboratories in a parasitic manner. With the growing demand for such radiation coming from many fields of science, new storage rings were designed and optimised exclusively for the production of such radiation. Today, more than 60 dedicated synchrotron radiation facilities are in operation throughout the world [1]. They have resulted in a number of totally new

Name	Perimeter (m)	Energy (GeV)	Current (mA)	Emittance (nm)	N. of ID Straight	Ring Commissioning
DIAMOND	560	3	300	2	24	2005
SOLEIL	354	2.75	500	3.1	24	2005
LLS	252	2.5	250	8.5	12	
SPEAR3	240	3	500	18	18	2002
CLS	171	2.9	500	18	12	2003
BOOMERANG	184	3	200	11.5	12	
SSRF	396	3.5	300	4.8	20	

Table 1: Main parameters of the future storage ring based synchrotron light sources under construction (in black, European sources).

scientific applications. Synchrotron radiation applications take place in several fields of science, such as physics, chemistry, biology and medicine but also in industry such as micro-electronics, pharmaceuticals, metallurgy, plastic materials. At present there are still more than seven storage ring type facilities

under construction and much more at project level. With the large demand of the protein crystallography community around 0.1 nm, all new facilities are specified for a reasonable brilliance at this energy while keeping to a medium cost. The electron energy is a major constraint on the spectrum of the X-ray produced as well as on the cost. Nearly all of the new sources are in the 2.5 to 3.5 GeV range with a ring perimeter of between 150 and 400 m. The main characteristics of several of them are listed in Table 1. All new facilities intend to generate hard X-ray undulator radiation using narrow gap in-vacuum undulators. The combination of small emittance and small apertures results in a short lifetime. To overcome this, the almost continuous topping up, pioneered at APS and SLS, is mandatory. In addition, topping up ensures a high stability of the electron and photon beams. Figure 1 presents a comparison of the spectral flux observed through an aperture on a beamline produced by an undulator on the future Diamond source and undulators on the ESRF. Clearly, the flux is one order of magnitude lower at 0.1 nm. The difference of flux and brilliance comes both from the lower energy and the use of a high undulator emission harmonic number. The hard

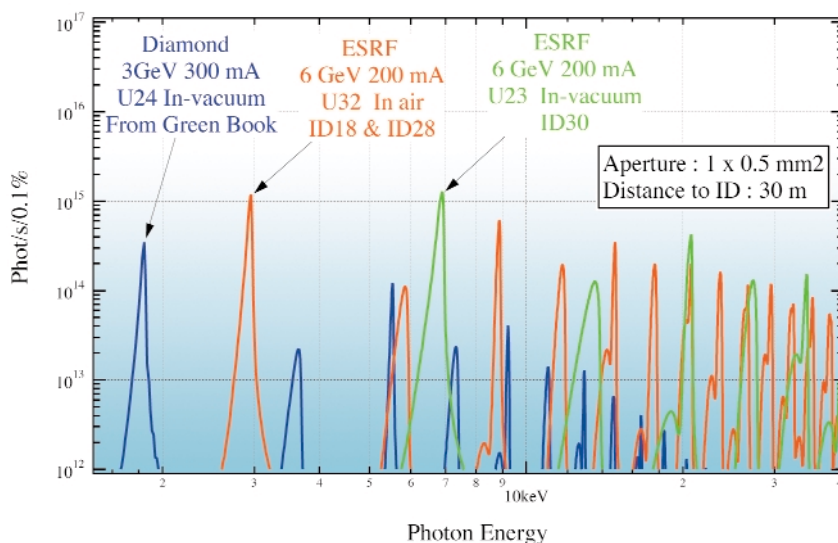


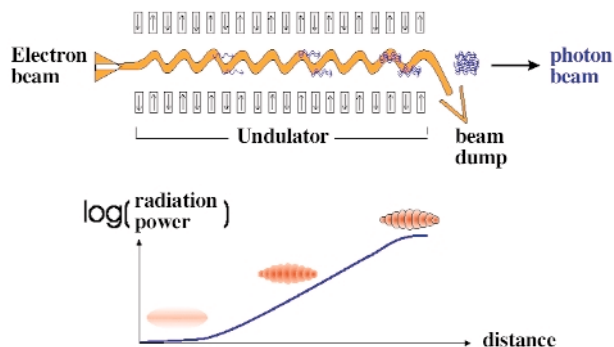
Fig. 1: Undulator spectral flux collected in a 1 x 0.5 mm² aperture at 30 m from the source produced by an in-vacuum undulator on the future Diamond source compared to that of an ESRF undulator. The ID18 or ID28 U32 undulators are presently in operation, the ID30 in-vacuum undulator U23 will be installed in 2003.

X-ray sources worldwide are the ESRF, the APS and SPring-8. They operate with a ring current between 100 and 200 mA and an emittance between 3 and 6 nm. A brainstorming is taking place within the ESRF machine division to identify what could be the parameters and the technological choices for an ultimate hard X-ray source. The parameters of the design presently under study are an energy of 7 GeV, a perimeter of 2 km, a current of 500 mA and an emittance of 0.2 nm. Such a source would provide a brilliance two orders of magnitude higher than that of the ESRF [2].

Linac with SASE

The Free Electron Laser (FEL) concept was invented by J. Madey and first operated in 1977 [3]. There are a number of facilities worldwide which provide tunable infrared radiation [4]. Unfortunately, the gain is usually low and these lasers are operated with an optical cavity. The cavities, made of normally reflecting mirrors, are suitable for the visible and infrared ranges but cannot provide enough reflectivity in the X-ray range. One way to eliminate this difficulty is to remove the mirrors and use a long undulator. The spontaneous emission (identical to synchrotron radiation) from an undulator is self amplified and, if the undulator is long enough, may reach the saturation level typically 6 to 7 orders of magnitude above the level of the synchrotron radiation (See Figure 2). Such sources require a high peak current of electrons as well as a very low emittance. While the concept was proposed nearly 20 years ago, it is only very recently, with the development of the laser-driven radio frequency electron gun, that the required beam quality could be reached by linear accelerators. Table 2 presents the status of development of SASE type sources. Three sources have reached saturation in the past two years, at APS (385 nm), BNL (830 nm) and Tesla Test Facility at DESY (90 nm). Note that the Tesla Test Facility (TTF) at DESY has demonstrated a GW peak power with pulse duration shorter than 100 fs. The three sources currently under construction or in the final design phase are the TTF2 facilities at DESY, the SPring-8 Compact SASE Source (SCSS) in Japan and the Linac Coherent Light Source (LCLS) at Stanford. The ultimate goal of a SASE source is a very bright 0.1 nm monochromatic beam. The requirements in beam quality and performance to run a 0.1 nm SASE type

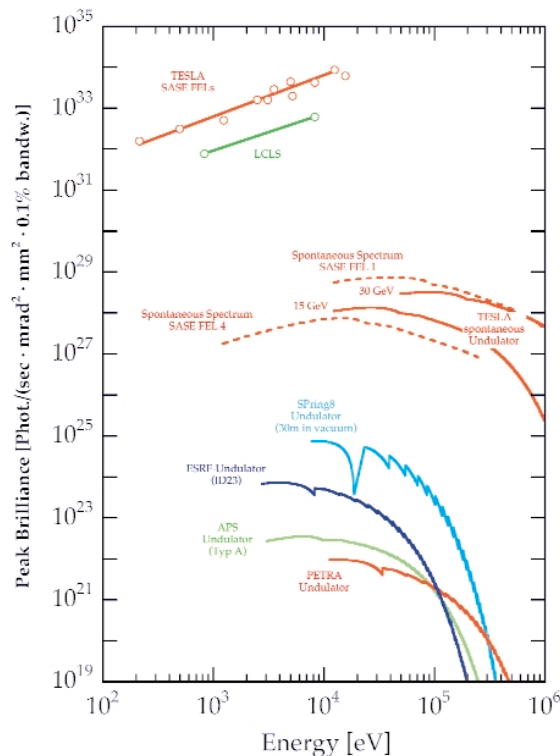
Figure 2: Principle of Self Amplified Spontaneous Emission. As the power grows during the propagation of the beam in the undulator, a longitudinal bunching of the beam takes place. (From the TESLA TDR Report).



Project	Status	Energy (GeV)	λ (nm)	Gap (mm)	Und. Length (m)	Commissioning
VISA [5]	Operation.	0.07-0.085	830	6 Fixed	4	2000
LEUTL [6]	Operation.	0.33	385	11 Fixed	30	2000
TTF-1 [7]	Operation.	0.23	90	12 Fixed	15	2001
TTF-2 [7]	Construction	1	6	12 Fixed	30	2004
SCSS [8]	Construction	1	3.6	3-5 Variable	25	2003 @ 15 nm 2005 @ 3.6 nm
LCLS [9]	Design	4.5-14	0.15	6 Fixed	120	2008
ELETTRA [10]	Planning	1	10-40	? ?	? ?	? ?
BESSY [11]	Planning	2.3	1	? ?	? ?	? ?
TESLA	Planning	25	0.085	10	< 320	2011
XFEL [7]				Variable	180	

Table 2: Main parameters of the SASE type light sources presently in operation, construction and design.

Figure 3: Peak brilliance of the Stanford LCLS and DESY TESLA future facilities compared with those of present hard X-ray synchrotron sources. (From TESLA CDR Report).



source are just on the edge of present technological capabilities. First the linear accelerator must have an energy of at least 15 GeV, however, 25 GeV is a more appropriate energy. Concerns are focussed on the gun design, which must

simultaneously deliver a high charge and a low emittance; the control of all accelerator components to preserve low emittance during transport; and acceleration. To reach a required peak current of 3-5 kA, several stages of bunch

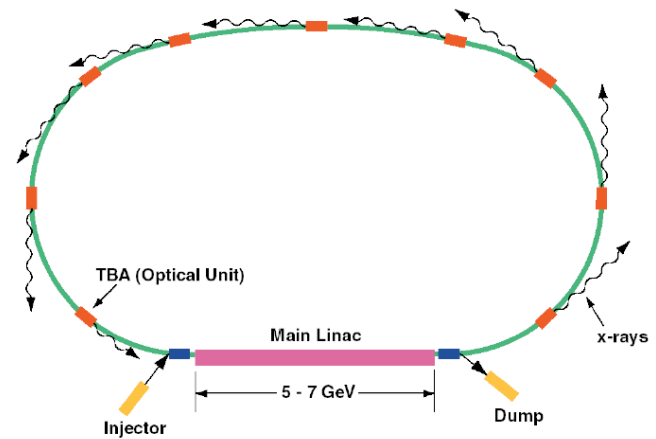
compression are needed along the acceleration path. Coherent synchrotron radiation is produced in the magnets of the bunch compressors which may damage the energy spread and emittance. Finally a very long undulator of 100 to 300 m in length is needed in which the trajectory must be controlled and aligned to an absolute precision of a few microns. At present there exists two proposals in the world to build a 0.1 nm SASE facility: the LCLS at Stanford; and the TESLA X-FEL at DESY. The goal of SASE type sources is a high brilliance together with a very short pulse. This is best illustrated by what is called “peak brilliance”. **Figure 3** presents the expected peak brilliance of the LCLS and TESLA X-FEL sources compared with existing storage ring type sources.

It is felt widely within the community that the type of science carried out in these facilities when they come into operation will be quite new. The focus there will be on ultra-fast science benefitting from short pulses, or applications requiring the huge power density. However, applications that need average flux and brilliance are more likely to be carried out on conventional storage ring based light sources.

Energy Recovery Linac

Linear accelerators have never been used as synchrotron sources because of the low average current that they produce which is the consequence of the non recirculation of the beam. Nevertheless, with the recent progress in the development of superconducting radio-frequency cavities, the concept of an Energy Recovery Linac (ERL) has emerged. An ERL can be thought of as a sort of ring in which the RF cavity has

Figure 4: Concept of an Energy Recovery Linac (from Cornell: <http://erl.chess.cornell.edu/>)



been expanded in order to be able to accelerate a beam from very low energy to the nominal full energy. If the cavity is superconducting, the field decay time in the cavity is long (a few milliseconds) compared to the time needed by the beam to make one turn (a few microseconds). As a result, the beam re-enters the cavity after one turn while the field remains and if its phase is π instead of 2π , with respect to the RF field, it is decelerated rather than accelerated, the energy is stored in the RF field in the cavity and used to accelerate freshly injected electrons coming from a low energy cw electron gun followed by a short linear accelerator (injector). This concept resembles the storage ring with the important difference that the electron energy is recirculated but not the electron itself (as in a storage ring). As a result, it is the injector rather than the balance between damping and excitation that determines the bunch length, energy spread and emittance of the beam as is the case in a storage ring. In other words, a very small emittance, short bunch, small energy spread beam can only last for a few milliseconds in a storage ring, beyond this the irreversibility of the process of emission

of synchrotron radiation forces the electron population to lose memory and reach a new statistical equilibrium. Since the beam in an ERL stays for one turn or possibly a few turns, this new equilibrium is never reached. It is believed that the average current in the 100 mA range should be sustainable. **Table 3** presents the various proposals of ERL worldwide. Some of the technological challenges associated with ERLs are the following. The high average current and short bunches dissipate a lot of power in the cavities and the existing best designs such as the TESLA type cavities cannot really be used without extracting the Higher Order Modes out of the cavity and dissipating them at room temperature. Such cavities are being developed for new high current synchrotron sources but with a more modest gradient and so far only produced at much lower frequencies. The gun and pre-injector must be able to sustain a continuous operation of 100 mA while present guns generate only a few milliamps. The presence of a halo around the beam combined with high current may generate safety issues. A new type of transverse instability is expected which is induced by the interaction of multiple bunches over multiple turns with the higher order modes of the accelerating cavity (multi-turn multi-bunch beam breakup). Following a first experimental investigation in 1987 at the Stanford Superconducting Accelerator in a free electron laser experiment, the proof of feasibility has been demonstrated at Jefferson Lab with a recirculated 5 mA 40 MeV electron beam in an experiment targeting a high power free electron laser. The concept has been largely advertised by teams in Novosibirsk [19] and Cornell University [20]. Contrary to the SASE which is a major change of technology compared to storage ring light sources, ERL appears more like an evolution, it makes use of the normal synchrotron radiation from undulators.

Name	Energy (MeV)	Current (mA)	Date	Remarks
Jefferson Lab. [12]	40	5	1999	For 10 kW cw oscillator FEL in I.R and UV
	160	10	2002	
JAERI [13]	15	5		For 1 kW cw oscillator FEL in I.R and UV
Cornell Univ. [14]	100	100		Target a multi-user facility with both high average current and short bunches
	5000	100		
BNL [15]	3000	Up to 200		NSLS upgrade
LBNL [16]	2500	0.01		Target a multi-user facility, femtosecond facility - 1 nC, 10 kHz, 50 fs
Daresbury Lab. 4GLS [17]	600	200		Cover IR to soft X-ray with many type of FELs
Univ. Erlangen [18]	3500	?		Consider the upgrade of a storage ring type facility with ERL capability

Table 3: Main parameters of the existing and planned ERL-type light sources.

References

[1] For the web site addresses of all existing and projected synchrotron sources see: http://www-ssrl.slac.stanford.edu/sr_sources.html.

See also the Shanghai Symposium on Intermediate Energy Light Sources. <http://ssils.ssrc.ac.cn/>

[2] A. Ropert, J.M. Filhol, P. Elleaume, L. Farvacque, L. Hardy, J. Jacob, U. Weinrich, "Towards the Ultimate Storage Ring Based Light Source", EPAC 2000 available at <http://accelconf.web.cern.ch/accelconf/00/PAPERS/TUZF101.pdf>

[3] D.A.G Deacon, L.R. Elais, J.M.J. Madey, G.J. Ramian, H.A. Schwettman, T.I. Smith, *Phys. Rev. Lett.* **38**, 892 (1977).

[4] See the Free Electron Laser World Wide Web Virtual Library:

http://sbfel3.ucsb.edu/www/v1_fel.htm

[5] <http://www-ssrl.slac.stanford.edu/VISA/>

[6] <http://www.aps.anl.gov/aod/mcrops/leut/>

[7] <http://tesla.desy.de/>

[8] <http://www-xfel.spring8.or.jp/>

[9] <http://www-ssrl.slac.stanford.edu/lcls/>

[10] <http://www.elettra.trieste.it/science/elettranews/volume44/en103.html>

[11] http://www.bessy.de/lab_profile/01.FEL/index.php

[12] <http://www.jlab.org/FEL/>

[13] Ryoichi Hajima, presented at the 24th Advanced ICFA Beam Dynamics

Workshop on Future Light Sources, May 1-4 2002.

[14] <http://erl.chess.cornell.edu/>

[15] <http://nslsweb.nsls.bnl.gov/nsls/org/PERL/>

[16] Zholents *et al.*, Proc. of the SRI2001 Conference, http://erl.chess.cornell.edu/SRI2001_proceedings/ZholentsMadisonWS.pdf

[17] <http://www.4gls.ac.uk/>

[18] <http://www.uni-erlangen.de/docs/FAU/fakultaet/natl/>

www.erlsyn.uni-erlangen.de/

[19] G. Kulipanov *et al.*, Proc. of the SRI2001 Conference

[20] http://erl.chess.cornell.edu/SRI2001_proceedings/mars1_kulipanov.pdf

ACCELERATOR RELIABILITY WORKSHOP

4-6 February 2002

A workshop dedicated to accelerator reliability was held at the ESRF from Monday 4 February to Wednesday 6 February. About 80 experts attended the workshop. This meeting brought together all accelerator communities: accelerator driven systems, X-ray sources, medical and industrial accelerators, spallation sources projects (American and European), nuclear physics, etc. With newly proposed accelerator applications such as nuclear waste transmutation, replacement of nuclear power plants and others, reliability has now become a number

one priority for accelerator designers. This aspect is now taken into account in the design/budget phase, especially for projects whose goal is to reach no more than ... 10 interruptions per year! The high-quality presentations given in the workshop inspired some very useful discussions. It soon became apparent that there is a need for a better exchange of information about equipment reliability, the technical problems encountered and the solutions adopted in the different Institutes. Therefore, it was decided to start a website dedicated to accelerator reliability which will



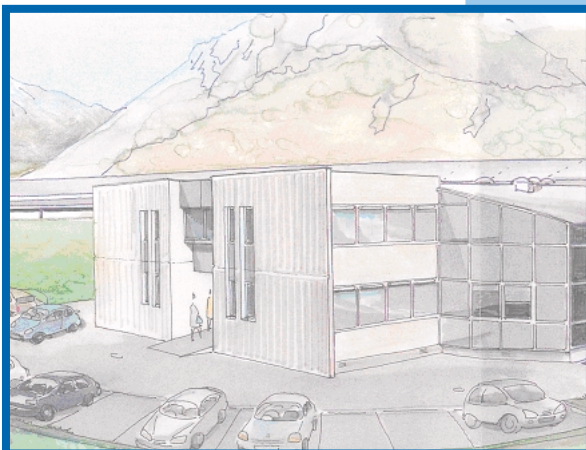
concentrate on technical information around that topic. The workshop ended with a visit of the various parts of ESRF equipment aimed at increasing reliability at the ESRF: the power supply commutation grid, the redundant RF system, the HQPS and ... the control room.

NEW COMPUTING ROOM

The computing needs of the ESRF progress rapidly and constantly. As the computing room in the Central Building was saturated, it therefore became essential to create a second computing room. This second room will have the advantage of ensuring that in case of incident the operation of the Machine and the beamlines will not be completely shut down. The obvious place to locate this new computing room was somewhere linking the Control Room with the Central Building.

In order to accommodate this request, the internal structure of the existing Control Room building will be modified and extended by a further 180 m² to allow the creation of this second computing room on the ground floor.

Works began in June 2002. At the time of going to press, the main works are being carried out and the heating, ventilation, air-conditioning and electrical works have just begun. The new premises will be available to users on 20 December 2002.



COLLABORATION WITH EIROFORUM

The ESRF and six other European intergovernmental (or multigovernmental) research organisations (EIRO) have set up a co-ordination and collaboration group (EIROforum) with their Directors General or equivalent as its members. A primary goal of EIROforum is to play an active and constructive role in promoting the quality and impact of European research. In particular the group will be a basis for interactions and co-ordination. Apart from the ESRF the participating organisations are the European Organisation for Nuclear Research (CERN), the European Fusion Development Agreement (EFDA), the European Molecular Biology Laboratory (EMBL), the European Space Agency (ESA), the European Southern Observatory (ESO) and the Institut Laue-Langevin (ILL). These organisations are committed to serve Europe's scientists by providing world-class research infrastructures. At the same time, they are fostering collaboration in science, both Europe-wide and in a world-wide context.

With the scientific, technological and project management skills of the organisations, the range of sciences that they cover and the magnitude of the financial investments involved, the EIROforum is an authoritative and representative actor in the current process of creating the European Research Area.

Aims of the EIROforum

- Encourage and facilitate discussions among its members on issues of common interest, which are relevant to research and development.
- Maximise the scientific return and optimise the use of resources by sharing relevant developments and results, whenever feasible.
- Co-ordinate the outreach activities of the organisations, including technology transfer and public education.
- Take an active part, in collaboration with other European scientific organisations, in taking a forward-look at promising and/or developing research

directions and priorities, in particular in relation to new large-scale research infrastructures.

- Simplify high-level interactions with the European Commission (EC) and enable an effective response to specific requests for expert advice in the areas covered by the member organisations.
- Provide co-ordinated representation to the outside world including the general public, national governments, non-European countries, etc.

Working Groups

The EIROs have set up a number of specialised working groups dealing with a wide range of issues of common interest among them, such as Outreach and Education, GRID, Instrumentation/Materials, Human Resources and Scientific Workshops.

Some of the current projects of EIROforum are presented below.

K. Witte

THE GRID

Data Transfer and DataGrid

Data transfer to the users in the member countries is an ongoing concern for the ESRF. With 5000 user visits every year an enormous amount of data is produced (~30 Terabytes for 2001), which needs to be transferred to the users institutes. There are many reasons why it is important that users can either transfer or access large data sets over the Internet:

- Smaller institutes, e.g. university groups, may neither have the funds to afford expensive tape devices nor the means to store all the data on disk.
- In fields like protein crystallography, we expect that in the near future users will not need or want to come to the ESRF in person, but will monitor the experiment on-line over the network and have their data processed with standard programmes on-site.

- International collaborations will require access to the same data sets simultaneously.

A European effort is required to stimulate a continuous evolutionary improvement to the networks for scientific data exchange. A medium-term option seems to be the European DataGrid, a project funded by the European Union with the aim of setting up a computational and data intensive grid of resources for the analysis of data coming from scientific exploration.

The main goal of the DataGrid initiative is to develop and test the technological infrastructure that will enable researchers and scientists to perform their activities regardless of geographic allocation. It will also allow interaction with colleagues from sites all over the world as well as the sharing of data and instruments on a scale previously unattempted. It will

devise and develop scalable software solutions and test beds in order to handle many PetaBytes of distributed data, tens of thousands of computing resources (processors, disks, etc.), and thousands of simultaneous users from multiple research institutions.

DataGrid is an ambitious project. It does not start from scratch in this challenge: it relies upon emerging computational GRID technologies that are expected to make feasible the creation of a giant computational environment out of a distributed collection of files, databases, computers, scientific instruments and devices. Although currently not participating actively in the DataGrid project led by CERN, ESRF will enter in the near future as an active partner in this project, via EIROforum.

R. Dimper

EUROPEAN ROUND TABLE

M OUTREACH AND EDUCATION

Mission statement

The EIROforum Working Group on Outreach and Education serves as a forum for co-ordination and co-operation of outreach activities of the organisations participating in the EIROforum, including public communication and education, to the mutual benefit of the partners. The main goals are:

- Support and enhance science literacy of the European public,
- Draw attention to the virtues and strengths of international collaboration within research.

Joint activities may take the form of:

- Dedicated programmes aimed at specific audiences, e.g. journalists, teachers, secondary school students, etc.
- Common public events,
- Media activities, including publications (in print and/or on-line).

It is an expressed aim of the group to intensify interaction with the relevant activities and programmes of the European Union, to achieve synergies and enhance the effects of such undertakings. By providing a useful bridge between the respective research communities of the organisations, the European Union and the citizens of Europe within the field of public communication of science, the activities of the Working Group should constitute a positive contribution towards the creation of the European Research Area.

Projects already carried out

Since the year 2000, the following projects involving some or all of the EIROFORUM partners have been carried out:

- Jan-Dec 2000 : Physics on Stage (Science Week 2000)
- Jan-Dec 2001 : Life in the Universe (Science Week 2001)
- Apr 2001 – Apr 2002 : Physics on Stage 2
- Jan-Dec 2002 : Couldn't be without it (Science Week 2002).

Proposals for the future

- Jan-Dec 2003 : Physics on Stage 3 (Science Week 2003)
- Nov 2003 onwards: European Science Teachers Initiative (ESTI)

ESTI

The European Science Teachers Initiative (ESTI) has been the primary concern of the working group during the past twelve months. This programme will support European science teachers by supplying them with up-to-date information about current research, innovative teaching methods and new educational tools, while also providing them with opportunities for close international interaction that have not been available before. The ESTI will be carried out in close conjunction with the Sixth Framework Programme.

D. Cornuéjols

The Round Table (R.T.) for Synchrotron Radiation and Free Electron Lasers held its annual meeting at the ESRF on 7 and 8 October. Representatives from the Members organisations (ANKA, BESSY, CLIO-LURE, DARESBURY, ELETTRA, EMBL-GRENOBLE, EMBL-HAMBURG, FOM, HASYLAB, ISA, LURE and MAX-LAB) were joined by members of the Round Table Coordination Group, a representative from the European Commission, and representatives from Users of R.T. facilities. Observers from the SLS and DIAMOND were present, while the ESRF, although not formally a R.T. member, acted as organiser and co-chair of the meeting.

After presentations on the different facilities and their participation in EC-funded R.T. activities, the discussion centred on the future of the Round Table in the context of the 6th Framework Programme (FP6). The RT delegates agreed to set up a working group to prepare a draft proposal for an integrated infrastructure initiative within FP6. We are pleased to note that the ESRF will be considered as a full participant in future R.T. activities. However, since the access funding, of importance to other R.T. members, is not appropriate for ESRF given its international status, this participation will probably be centred on other types of collaborations such as instrumentation or communication.

W.G. Stirling

INSTRUMENTATION AND MATERIALS

The most important common factor of the EIROs is that they are all committed to provide the European scientists with world-class experimental facilities. As a consequence, the EIROs are continuously working at the frontiers of instrument research and development. The EIROs have in the past profited from each others developments, either indirectly or through collaborative projects. The mission of the working group on instrumentation and materials is manifold. The first mission statement is to raise the awareness within the EIROs of the know-how and expertise available within the other EIROs. The

second task is to look into ways how the expertise in one EIRO can be transferred to another EIRO. The third goal is to identify projects common to two or more EIROs. The fourth and final goal is to develop a view of future needs and perspectives in instrumentation.

Each member of the working group collated a document describing their specific institute from the instrumentation point of view, including the ongoing developments and future needs. Subsequently the working group met on the 29 November 2001 at CERN. The main conclusions of this meeting was that there is indeed a large

overlap between the needs and requirements of the various EIROs in the field of instrumentation. The highest priority is clearly the development of improved two-dimensional detectors. The ESRF, being one of the main driving forces behind this, will organise a topical workshop on this issue in the near future. In the mean time a proposal for the development of pixel detectors is being worked out to be submitted under FP6, including CERN, EMBL, ESRF and possibly EFDA/JET. The ESRF is again taking a leading role in this initiative.

H. Graafsma

TENTH ANNIVERSARY OF THE BEAM

1st March 2002 coincided with the 10th anniversary of the first storage of electrons in the ESRF ring. To celebrate this event, an informal seminar was organised. There were presentations by R. Haensel, Y. Petroff, A. Ropert and P. Elleaume recalling the history of the construction of the Machine and the gain in performance levels over these ten years.



NEW DIRECTORS

New Research Director

On Monday 1st October 2001, Francesco Sette began his 5-year term of office as one of the ESRF's Research Directors, succeeding Christof Kunz. For more than 10 years he was Head of the Inelastic X-ray Scattering Group at the ESRF. Before he joined the ESRF, he was a staff member (1984-1990) at ATT Bell Laboratories (Murray Hill, NJ, USA). At SSRL (Stanford Synchrotron Radiation Laboratory, Stanford, CA, USA), NSLS (National Synchrotron Light Source, Upton, NY, USA) and finally at the ESRF he has worked on the development and improvement of synchrotron radiation



Francesco Sette

instrumentation in order to perform X-ray spectroscopy with high-energy resolution.

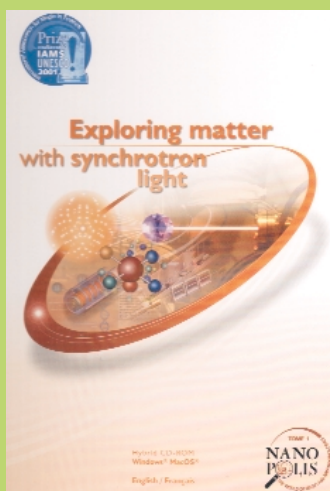
New Director of Administration

Starting on Tuesday 2nd April 2002, Helmut Krech succeeded W.E.A Davies as Director of Administration. H. Krech, 58 years old, pursued legal studies in



Helmut Krech

Germany and France. His doctoral thesis dealt with French public law. He worked in the legal departments of the Karlsruhe Research Centre and the German Development Company. From 1985 to 1989 he was Administrative Director and Deputy Chairman of the Board at Bessy and, since 1989, he held the same positions at DESY.



CD-ROM

The CD-ROM "Synchrotron light to explore matter" received the international IAMS Prize for the best scientific multimedia in 2001. Conceived for a worldwide audience of students, scientists and industrialists, the CD-ROM invites you to participate in a virtual tour of a synchrotron, it explains how a synchrotron works and covers its numerous applications. The CD-ROM is now distributed by ImediaSoft and ESRF under the title "Exploring matter with synchrotron light". More information can be found on the website : <http://synchrotron.imediasoft.fr/indexEN.htm>