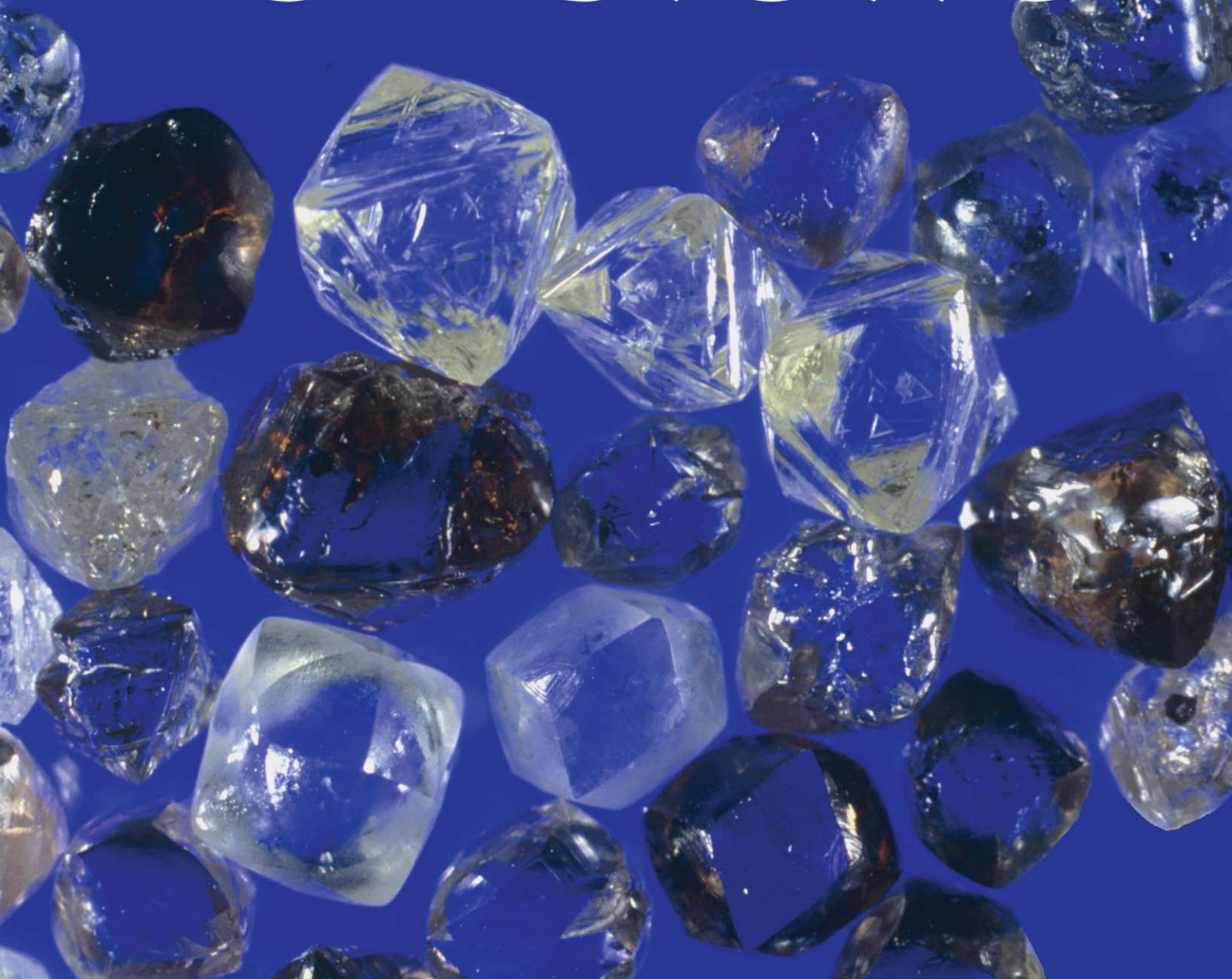


# ESRF Newsletter



**Diamonds play  
the ace in research**





Editor: Montserrat Capellas Espuny  
European Synchrotron Radiation Facility BP220,  
F-38043 Grenoble cedex; tel: +33 476 88 26 63;  
e-mail: press@esrf.fr

Editorial committee: Nick Brookes, Dominique  
Cornuéjols, Pascal Elleaume, Andreas Freund, Axel  
Kaprolat, Sine Larsen, Sean McSweeney, Francesco  
Sette, Bill Stirling and Karl Witte

Photographer: Chantal Argoud

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Publisher: Jo Nicholas

Production: Kate Boothby

Technical Illustrator: Alison Tovey

Display advertisement manager: Chris Thomas

Advertisement production: Teresa Honey, Tanwen Haf

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Not just a focus of admiration. The ESRF uses synthetic diamonds in single-crystal form as monochromators. See p4.

## Contents

### Editorial

- 3 The ESRF and Europe share a vision

### Feature news

- 4–5 Diamonds play the ace in research  
6–7 Bacterium aids study of nitric oxide  
9–10 Was Agnès Sorel – the first official royal  
mistress of France – really poisoned?  
13 EIROforum promotes a single European market  
in science  
15 MPI builds a unique spectrometer  
15 Hubert Curien 1924–2005

### Interview

- 16–17 Elizabeth Moulin: personality assessor

### Scientific highlights

- 19 X-ray absorption, refraction and resonant  
scattering tensors in selenated protein  
crystals  
20 Direct observation of giant d-band splitting in  
holmium  
21 Small-angle X-ray scattering of a supercritical  
electrolyte solution: the effect of density  
fluctuations on ion hydration  
21 Smoothing of tungsten films by ion polishing  
22 New possibilities at ID10B: high energy for  
surface studies at liquid/liquid interfaces  
22 Probing vibrational excitations in molecular  
crystals by inelastic X-ray scattering: from  
neutrons to X-rays

- 23 Simultaneous tomography and diffraction  
analysis of creep damage

### Technical article

- 24–25 Why Infrared spectromicroscopy at the ESRF?

### User's view

- 26–27 Serena Margadonna – winner of the 2005 ESRF  
Young Scientist Award

### Visiting a beamline

- 28 Macromolecular Crystallography Group has  
new baby

### Gallery of events

- 29–30 Course aims to make knowledge in X-ray and  
neutron techniques stronger  
30–31 The ESRF celebrates its 15th Users' Meeting  
31 Satellite workshop: synchrotron radiation in  
art and archaeology  
31 Satellite workshop: new science with new  
detectors

**The ESRF and Institute of Physics Publishing have formed a new partnership to produce *ESRF Newsletter*. From this issue Institute of Physics Publishing will publish *ESRF Newsletter* under contract. The ESRF will provide editorial content and retain editorial control, while production, advertising sales, printing and distribution will be handled by Institute of Physics Publishing. Institute of Physics Publishing is an experienced STM publisher and publishes a portfolio of magazines, including *Physics World* and *CERN Courier*.**



# Editorial

W.G. Stirling, Director General

## THE ESRF AND EUROPE SHARE A VISION

In December 2003 I wrote about the participation of the ESRF in the EIROforum, which unites seven major European intergovernmental research organizations. I discussed the development of the European Research Area (ERA) in the context of the Lisbon and Barcelona goals to develop a knowledge-based economy for Europe. Since then there have been major developments, including the definition of the 7th EC Framework Programme (FP7) and a refinement of the ERA.

EIROforum has recently produced the document "Towards a Europe of knowledge and innovation", in which the partners describe their vision of the future of scientific research in Europe, with emphasis on large research infrastructures, like the ESRF. The paper was launched at a ceremony in Brussels on 20 April, with the participation of the new European commissioner for science and research, Janez Potočnik, and the minister of culture, higher education, employment and research of Luxembourg, François Biltgen (page 13).

Continuing the Europe theme, the ESRF is involved in many collaborative research projects, funded by the European Commission, within FP5 and FP6. Along with all major synchrotron radiation (SR) and free-electron laser centres, it is a member of the Synchrotron Radiation Round Table (SRRT). The SRRT's annual meeting was held at Bessy in 2005. Probably its most important activity is to coordinate the EC funding

that supports access by European scientists to 13 member laboratories.

The ESRF is not a recipient because funding comes directly from its member and scientific associate states, but it is actively involved in Joint Research Activities (JRAs) as part of an EC Integrated Infrastructure Initiative. As their name suggests, JRAs combine expertise and experience from SRRT laboratories to tackle scientific and technical problems of common interest.

### ESRF takes the lead

Crucially, we are lead laboratory for a project to design, develop and test a superconducting undulator. This will open up exciting research possibilities for medium-energy SR sources by extending exploitable X-ray energies into the 50–100 keV range and strengthening the ESRF's hard-X-ray capabilities.

Networking is another SRRT activity supported by the I3 – workshops, conferences and schools with ESRF staff will benefit from EC funding, and structures are being developed to favour the transnational exchange of scientists.

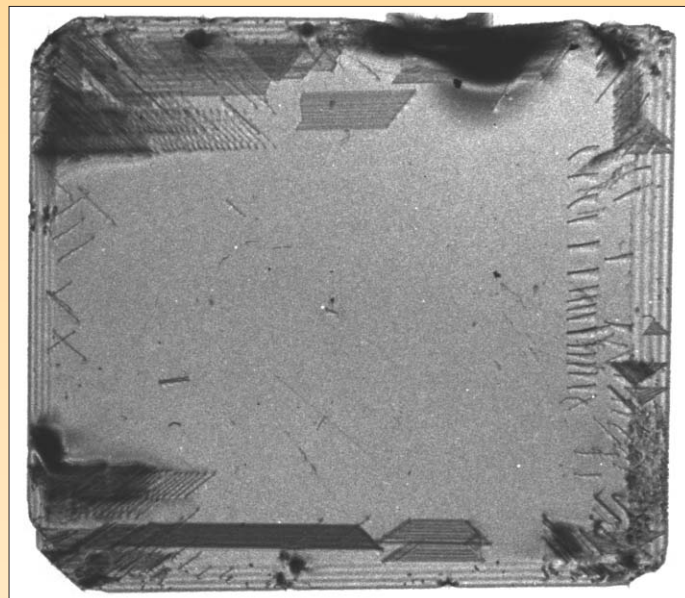
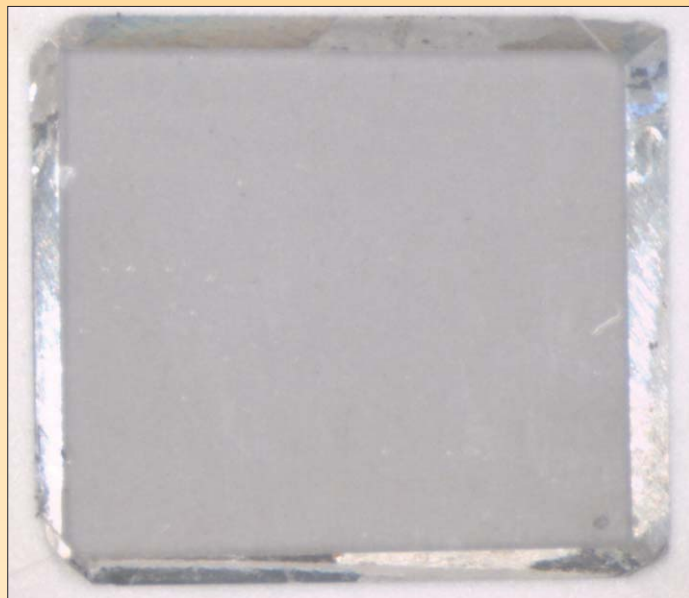
The ESRF's scientists have been successful in obtaining funding under FP5 and FP6. In the past year a new batch of FP6 contracts have begun. In many cases an ESRF staff member acts as project coordinator. The contracts involve a range of laboratories and universities (e.g. the Materials Science Project on ductile bulk metallic glass composites involves 12 institutions,

mostly in ESRF member countries). The FP6 contracts cover various kinds of science from ultrafast time-resolved diffraction to ion implantation in semiconductors. Preparations for FP7 are well advanced and more emphasis on fundamental research is expected. The ESRF's scientists are working with their colleagues across Europe to prepare for the new EC programme.

I should like to extend these considerations on exchange and collaboration outside Europe. Communication is key in research, and one of our most effective tools is the Internet. Light sources across the world have combined to create a website for the international light source community – [lightsources.org](http://lightsources.org). Research at synchrotron and linac-based light sources is one of the most dynamic fields of science, often resulting in direct benefits to society. But this is not widely appreciated outside the scientific community, or even outside the immediate SR user community. The aim of the site is to establish effective communication between experts at the world's light sources and thus maximize the impact of communication activities at these facilities.

Multiple audiences need to be addressed. The website will provide information of interest to them all. On behalf of the ESRF and of our users, I should like to congratulate the organizers of this important initiative. I am sure we will all benefit from visiting this innovative site.

## Feature news



**Diamonds are forever.** Optical micrograph (left) and white beam X-ray topograph (right) of a highly pure type IIa crystal. The topograph (taken in transmission geometry) shows extended dislocation-free and homogeneous areas in the central part.

## DIAMONDS PLAY THE ACE IN RESEARCH

**Diamonds are rare gems that are meant to be seen. However, these stones made of pure carbon are not just a focus for admiration. This is the story of how, hidden from human eyes, they can be extremely useful.**

**Y**ou could stare at them for hours. Their appearance captivates anyone who gets the chance to observe one or have it placed on a finger. But behind their beauty lies a tool of great importance to synchrotron radiation facilities. For example, the ESRF uses them, in single-crystal form, not to decorate the synchrotron but to make it more efficient, thanks to diamond's many extreme properties, such as its low X-ray absorption, low thermal expansion and high thermal conductivity.

The first diamonds had their genesis under the surface of the Earth in conditions of extreme temperature and pressure some 3 billion years ago. They were brought to the Earth's surface much later, approximately 140–90 million years ago, via deep-seated gas-driven volcanic explosions. They were then transported in a solid breccia known as kimberlite. This is the type of primary deposit where rough diamonds can still be found today. Some of them became eroded out of the kimberlite and were distributed into rivers and along coastlines. Humans first discovered these gems around 4000 years ago.

According to the American Museum of Natural History, some 80% of natural diamonds are used in industry because they contain flaws or impurities that result in poor optical

qualities, so they are unsuitable for use as jewellery. About four times the production of natural diamond for industry is actually grown synthetically. That makes a total of more than 500 million carats or 100 000 kg.

The hardness of the diamond makes it perfect for industry for use in abrasives or as surgical blades, which need to cut very precisely. They are even used in the space industry where they are drilling Mars for the first time.

### Between a rock and a hard place

How can the hardest natural substance ever known be made artificially? The single-crystal diamonds used at the ESRF were grown during several weeks in a high-pressure, high-temperature environment to reach a size of almost 1 cm<sup>3</sup>.

At the ESRF, synthetic single diamonds are used mainly as X-ray monochromators. Their main advantages are that they can withstand high temperatures almost without deformation because of their low absorption and low thermal expansion, and because they have the highest heat conductivity ever known.

The ESRF was in fact the first synchrotron radiation institute to use this gem as a monochromator. "At the beginning, no-one knew how to handle these powerful beams that we





**Diamonds are a scientist's best friend.** A meeting about projects with diamonds took place at the ESRF last May. It brought together staff from the University of Witwatersrand (South Africa), Element Six (De Beers Industrial Diamonds) and the ESRF. Upper row, left to right: Rhyme Setshedi (University of Witwatersrand), Joanna Hoszowska (ESRF), Pierre Van Vaerenbergh (ESRF), Mik Rebak (University of Witwatersrand), Herman Godfried (E6), Toon Sturm (E6), Manuel Rodríguez Castellano (ESRF), Joh Hansen (E6). Lower row: Jürgen Härtwig (ESRF), Simon Connell (University of Witwatersrand), Robbie Burns (E6), Denson Dube (University of Witwatersrand), Lucky Mkhonza (University of Witwatersrand), Isabella Gierz (ESRF).

get at the ESRF, so we came up with the idea with Jens Als-Nielsen and we did tests in 1992 on the diamonds. It turned out to actually work!" explained Andreas Freund, former head of the optics group. This was simultaneously confirmed at Brookhaven National Laboratory. This was the starting point for a long collaboration with Element Six, which is the world's premier diamond company, through Friedel Sellschop, now deceased, but then vice-chancellor of the University of Witwatersrand, South Africa.

There are five diamond monochromators installed on beamlines at the ESRF: three on ID14 and two on ID10. Each has a value of around €15 000. The more widespread use of diamond has awaited a research programme, which is a collaboration of diamond growers, synchrotron scientists and diamond physicists. That programme has now been initiated at the ESRF, and it has already led to spectacular improvements in diamond quality, such as the very low strain and essentially defect-free sample shown above. This is very exciting for improved X-ray beams at synchrotrons.

The ESRF also pioneered the use of diamonds as transmission phase plates because they modify the polarization state of X-ray light.

Today, the three biggest synchrotron facilities in the world

(ESRF, APS and Spring 8) use synthetic diamonds as monochromators. These will play an even more important role in the future. Practically, diamond is the only material that can be used as a monochromator in free electron X-ray lasers – the next generation of light sources. The aim of scientists at the ESRF and the synthetic diamonds' manufacturers is to improve their quality, even though they are already much better than at the beginning of the collaboration. Perhaps they succeed in creating the perfect diamond. "It's definitely a big challenge," said Freund.

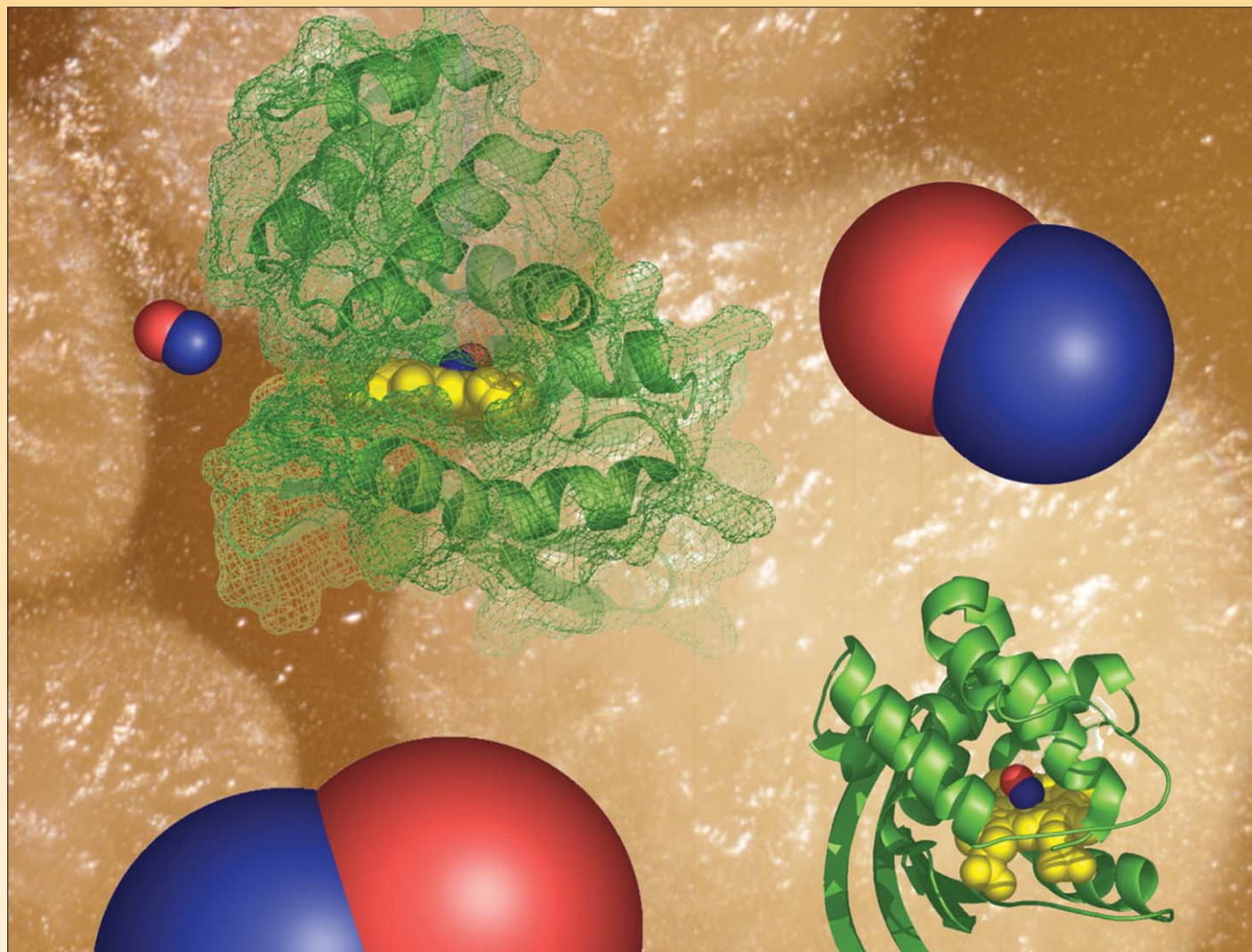
●  
MC

## ERRATUM

The caption of the photo on page 4 of the December 2004 issue was incorrect. It should have read:

"The white beam generated by a wiggler on ID11. This photo, which has been used in posters, magazines and other publications worldwide to illustrate synchrotron radiation, was taken by M Krumrey on 22 February 1993."

We apologise for any inconvenience that this error may have caused.



SONO binds to NO. Blue (nitrogen) and red (oxygen) spheres joined in the middle correspond to nitric oxide. SONO is represented as green.

## BACTERIUM AIDS STUDY OF NITRIC OXIDE

Researchers from Texas have used a bacterium to investigate the behaviour of nitric oxide in humans in relation to impotence and vascular disease.

A team from the Medical School at the University of Texas in Houston, US, has discovered more about the mechanism of action of nitric oxide (NO), which is produced widely in the body. It has been able to study the molecule thanks to the use of synchrotron light produced at the ESRF. The gaseous molecule is responsible for relaxing blood vessels in smooth muscles, such as those in the penis. By studying a closely related protein in bacteria, the researchers have identified how the human protein works.

Erectile dysfunction affects around 150 million men worldwide (2004 *Aviat. Space Environ. Med.* **75**(11) 997–1000). This pathology is due to decreased NO production. The main action of drugs like Viagra and Cialis is related to modification of NO signal pathways in the body. The molecule

mediates many physiological actions, including penile erection, kidney function and uterine contractions at birth.

The action of NO is mediated by the protein sensor guanylyl cyclase (sGC). When the sensor binds to NO, it catalyses the conversion of guanosine triphosphate to cyclic guanosine monophosphate (cGMP). This triggers relaxation of the blood vessels. Unfortunately, NO isn't always produced (as in the case of erectile dysfunction), leading to a lack of cGMP. This occurs when an enzyme called phosphodiesterase-5 breaks down cGMP. Drugs like Viagra and Cialis stop the action of phosphodiesterase-5.

The big question is: How does NO activate sGC? Looking for an answer, the University of Texas team came to the ESRF to study a bacterial protein with striking similarities to sGC. Efforts to study human protein have been hampered for nearly 30 years by the fact that the protein is difficult to handle or purify. However, by studying the closely related bacterial protein, scientists gain the same insights as they



## THE AVERSION OF CLOSTRIDIUM BOTULINUM TO NITRIC OXIDE

Botulism is caused by toxins made by some members of the *Clostridium botulinum* group. The toxins affect people by preventing certain nerves from functioning, resulting in muscle paralysis. A few nanograms can kill a human and botulism often results from eating contaminated food.

*C. botulinum* finds nitric oxide (NO) toxic. Thus it has no reason to produce its own NO and it also needs a mechanism to detect it. Owing to the toxicity of NO to the organism, *C. botulinum* harbours a protein called SONO that has exceptional affinity for NO and signals the presence of NO. In *C. botulinum* NO is toxic because it binds to and blocks several components of its respiratory system and so kills it.

Some bacteria generate NO from nitrite during a mode of respiration called denitrification. This explains the old practice of curing meat with nitrites to avoid botulism. In the US, nitrite curing has been approved by the Food and Drug Administration since 1925. In Europe, meat and cheese curing with nitrite and nitrate has been performed since the late 1800s.

would by studying the human protein. The bacterium, *Clostridium botulinum*, is the etiological agent of botulism and harbours a NO-sensing protein (SONO), which closely resembles sGC in humans. SONO has extremely high affinity for NO. The team determined the 3D crystal structure of SONO, using X-rays generated at ESRF beamline ID29. "The key consequences of this discovery is that, by determining the crystal structure of SONO, we now know what sGC looks like. Vascular diseases are a major problem worldwide. In many cases the inability to relax blood vessels is to blame. This means that sGC function is affected when NO is not produced in abundance. So, knowing the crystal structure of SONO – and thus sGC – helps with the design of activators for sGC. Thus we may be able to come up with strategies to intervene therapeutically in several vascular disorders," said Dr CS Raman, leader of this research.

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## References

P Nioche *et al.* 2004 Femtomolar sensitivity of a NO sensor from *Clostridium botulinum*, *Science* 306.



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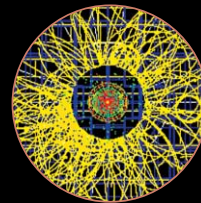


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Image: Prototype display of a simulated event, courtesy of the ALICE collaboration.

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#### Poisonous past?

The painting *La Vierge à l'Enfant* by Jean Fouquet. It is said that the model for the Virgin was Agnès Sorel, King Charles VII's mistress.

## WAS AGNES SOREL – THE FIRST OFFICIAL ROYAL MISTRESS OF FRANCE – REALLY POISONED?

The ESRF has gone back in time to try to reveal the reason behind the sudden death of the beautiful mistress of France's King Charles VII in the 15th century. X-rays of her hair and skin may provide some of the answers.

**T**hanks to synchrotron light, pieces of Agnès Sorel's hair and skin have been studied to try to determine the cause of her death. The evidence that has been gleaned makes it possible to suggest plausible causes of death. The way she died is not yet known but incredibly high levels of mercury have been found in her remains. This opens the door to numerous hypotheses. The corpse of Agnès Sorel was exhumed last September in Loches, France, to carry out this research.

The history of Agnès Sorel would make an excellent plot

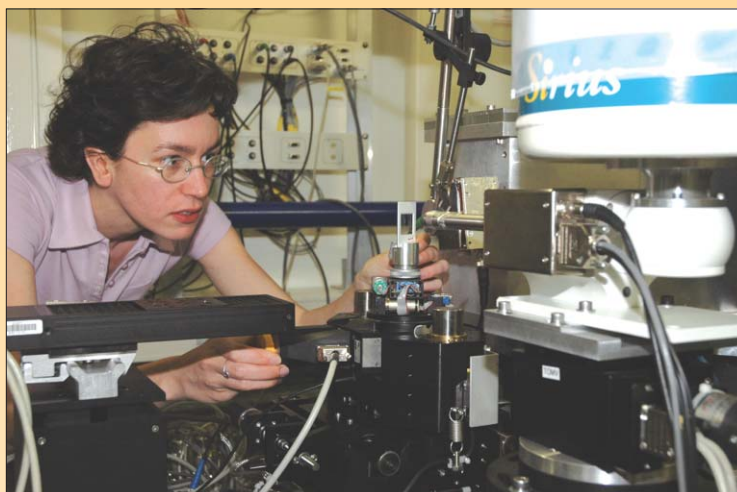
for a soap opera. She was the first mistress of a French king to be officially recognized as such. It is said that she was an extremely beautiful woman, as well as being very intelligent. She wielded considerable influence over the king and his policies, which earned her a number of powerful enemies at court. She gave birth to three daughters and, while pregnant with her fourth child, she joined Charles VII on a campaign against the English in 1450 in Jumièges, Normandy. Shortly afterwards, she fell ill and died of "flux of the stomach", according to the official account of events. However,



many believed that she had been poisoned because of her sudden death and numerous enemies.

Agnes Sorel's death was premature: she would have been only about 28 years old. To clarify the cause of her early demise, a team led by Dr Charlier from the CHU hospital in Lille is studying her remains through a variety of techniques. Samples of her hair and skin have been examined in minute detail using the X-rays of the ESRF. They have unveiled some indications that could lead researchers to discover the cause of Sorel's death. X-ray microfluorescence experiments were performed on beamline ID18F at the ESRF. Scientists found that her remains contained abnormal levels of mercury.

This element appears in the bodies of those who have been poisoned. However, one should avoid premature conclusions. Mercury is also present in pharmaceutical purgative



**Getting under the skin.** Marine Cotte, one of the ESRF's researchers who carried out the experiments using samples of Sorel's hair and skin.

treatments. Scientists found eggs from worms in other parts of her body, as well as remains of a plant used during that period to treat the worms. This could indicate that she was trying to heal herself by taking medicines and that she ingested too high a dose, which caused her death. Other possible sources of mercury contamination are the result of mummification or con-

tamination from the mummy's environment. She could also have accumulated the metal throughout her life by, for example, using cosmetics, since these often contained mercury.

In addition to the historic interest of this research, it also has consequences today: "Our research validates the medical and legal techniques that are used in criminal investigations," explained Charlier.

MC

## Photonic Science

### Making best use of beam time

Detector design is a compromise between speed of acquisition, detection area, linearity of response and signal to noise ratio.

Incorporating all these factors in one device means a modular detector design with parallel read out, 100% duty cycle, optimized Point Spread Function and high dynamic range.

Photonic Science's new Very High Resolution X-Ray VHR system combines all those features into a flexible design, and hence introduces a new way of acquiring dynamic diffraction patterns.

Because it allows simultaneous exposure/read out cycles, the camera delivers better sensitivity than other CCD systems when short duty cycles are required, as other systems are limited by dead read out time periods.

The camera provides > 100 times antiblooming suppression, thus avoiding bleeding artefacts that currently affect other CCD systems when high intensity peaks are neighbouring very low intensity ones.

The camera also eliminates the need for an external mechanical shutter, which means that it does not suffer from the frame shift smear that currently corrupts data quality of traditionally designed cameras during fast acquisition sequences.

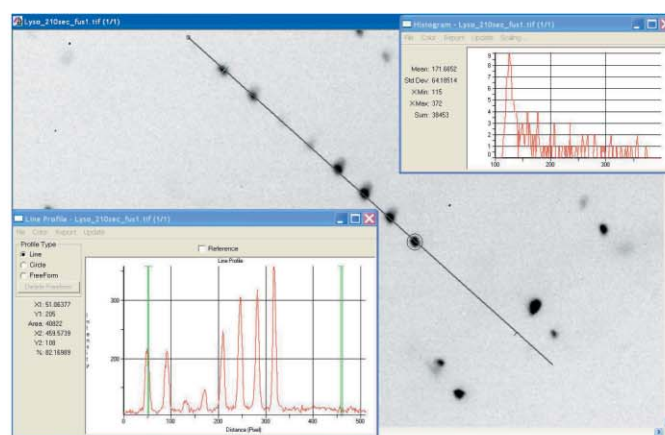
The camera delivers genuine 16-bit dynamic range data without the need of binning, thus solving the current dilemma between dynamic range and resolution.

Optimizing the Point Spread Function starts with a small pixel size, with custom phosphor deposition across its entire sensitive area. This makes the camera performance comparable to that of larger CCD cameras with poorer resolution set at a larger distance from the sample.

Low noise operation at 10MHz with multiplexed data output allows both fast and traditional long exposures for weakly diffracting proteins, small molecules, powders, organic and inorganic materials.

Integration within any existing diffraction set up can be achieved as simply as one would replace a mechanical shutter: providing a simple Low Voltage TTL pulse for setting exposure time or with a comprehensive Software Development Kit and Application Programmer's Interface (Linux and Windows platforms).

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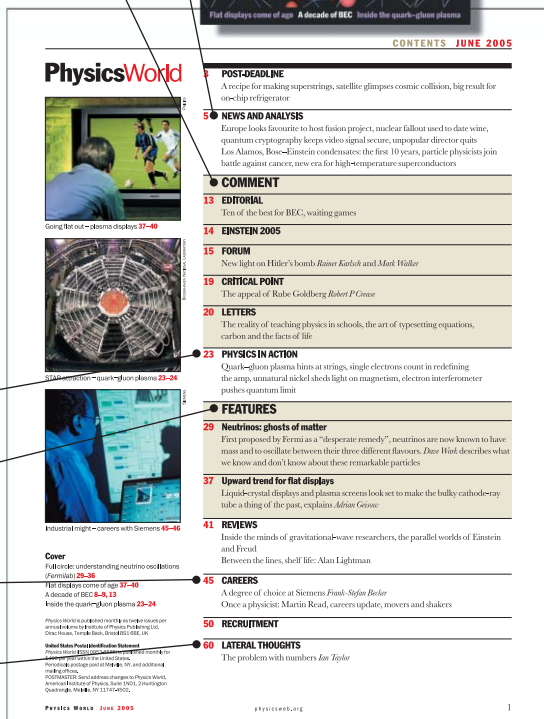
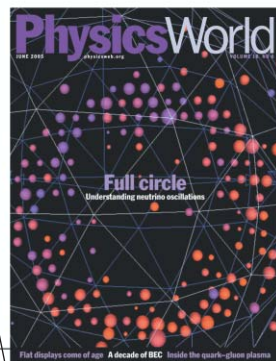
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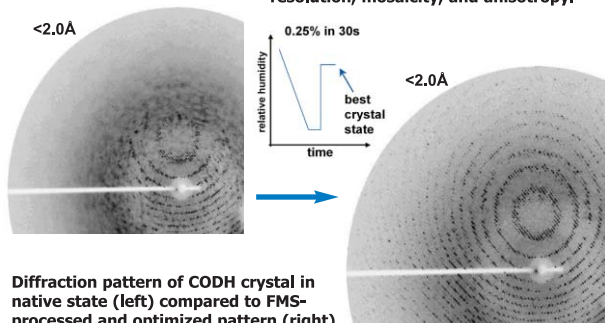
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# EIROFORUM PROMOTES A SINGLE EUROPEAN MARKET IN SCIENCE

European science “heavyweights” offer their help in the development of a knowledge-based economy, presenting a vision paper to the European Commission.

Europe’s seven major intergovernmental research organizations, working together in the EIROforum partnership, presented in April their paper on science policy, “Towards a Europe of knowledge and innovation”, in the presence of the European commissioner for science and research, Janez Potočnik, and the Luxembourg minister for culture, higher education, employment and research, François Biltgen. Luxembourg held the presidency of the European Union (EU) at the time.

Five years ago, at the meeting of the European Council in Lisbon, the creation of a European Research Area (ERA) was proposed as a means to achieve the ambitious targets necessary to develop a leading, knowledge-based economy in Europe. The ERA intends to make a single market for European research, bringing together scientists from all member states. The EIROforum partners operate some of the largest research infrastructures in the world, possess unique and long-standing expertise in the organization of pan-European research, bring expert knowledge to discussions about new large facilities in Europe, provide a model for the ERA, and offer their experience and active engagement in creating a true ERA.

## A vision for the future

The EIROforum paper describes the group’s vision on the future of European scientific research. It aims to support the Lisbon Process by working, alongside the commission, to implement the ERA. “As the borders of the EU expand, there is a fundamental role for the EIROforum partnership to work with the institutions of the EU in the evolving environment,” said Jean-Jacques Dordain, director general of the European Space Agency (ESA), which currently chairs EIROforum. The paper presents ways in which EIROforum organizations can participate in consolidating the ERA.

Attracting more young people is vital for the future of European research, and the paper offers a series of actions to stimulate their interest in science. It also subscribes to the European Commission strategy to recruit and retain



Sharing a vision. European commissioner for science and research, Janez Potočnik, speaking at the launch of the EIROforum paper.



Promoting knowledge and innovation. The seven EIROforum organizations were represented by their directors at the launch.

world-leading scientists in Europe. This should be supported by a European Research Council acting as an autonomous, science-driven agency endowed with sufficient funds to ensure that European research is competitive globally.

The EIROforum partners could also join European industry in technology platforms or large integrated projects that would enable the development of new scientific instrumentation – an area that needs European suppliers to secure and promote frontline research in Europe and generate important industrial spin-offs.

EIROforum is a partnership created in 2002 between CERN, EFDA-JET, EMBL, ESA, ESO, ESRF and ILL – seven of Europe’s major intergovernmental research organizations. The combined budget from the seven is comparable to that of the current Framework Programme of the EU. Each organization has become a world leader establishing an ERA within its own field of science, thereby demonstrating the value and feasibility of pan-European collaboration in research. “The EIROforum organizations present visible proof that Europe and Europeans working together can achieve more than any individual national effort,” said Jean-Jacques Dordain. ●

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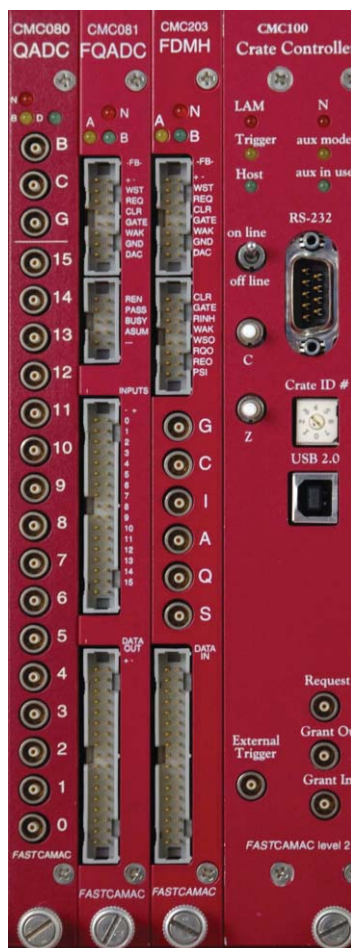
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Long stay results in a new arrival. Harald Reichert from the Max-Planck Institute explains how the new spectrometer works.

## MPI BUILDS A UNIQUE SPECTROMETER

Users from the Max-Planck Institute for Metals Research install a surface and interface diffraction endstation.

When users come to the ESRF, they normally stay for three or four days: they arrive, they do their experiment and they return with all of their data to their home institute. The team from the Max-Planck-Institute for Metals Research in Stuttgart is an exception. This winter they spent six weeks at the synchrotron, not only to carry out experiments but also to install a unique diffraction endstation on the High Energy Scattering Beamline, ID15. Thanks to this new spectrometer, scientists will be able to obtain high-resolution diffraction data, both from surfaces and from deeply buried interfaces.

The ESRF is the only place in Europe where this instrument can be used, because it needs a brilliant high-energy X-ray source. The instrument can be used in two different modes, where either the sample or the incident beam is moved to change the diffraction angles. Specially developed optics can keep the samples fixed while moving the incident beam. This option turns the instrument into a liquid spectrometer, which can reach very high vertical momentum transfer.

The device took the team six months to build. First they developed a prototype (to a scale of  $\times 0.1$ ). Although the prototype was delicate, the researchers were then able to test it and obtain results that have already been published. The spectrometer is now available to ESRF users.

●

MC

## HUBERT CURIEN 1924–2005

Prof. Hubert Curien died on 6 February 2005 aged 80. He began his scientific career as a specialist in crystallography and mineralogy. Later he was successively director of the CNRS, director of the Centre National d'Etudes Spatiales, president of the European Space Agency, French minister of research and technology (twice) and president of CERN Council. On several occasions he helped to advance the ESRF project.

Curien was at the origin of the European Science Foundation (ESF), set up in 1974. It fostered European collaboration in synchrotron radiation research. Under its auspices, several studies on a possible European synchrotron radiation facility were undertaken. However, at a point when these risked getting bogged down, Curien, who had been appointed ESF chair in November 1980, provided fresh impetus by suggesting the creation of an intergovernmental "Progress Committee concerned with the ESRF". This enabled further studies and served as a forum for the ongoing discussions on the political side, which resulted in the French-German decision to build the ESRF in Grenoble.

The memorandum of understanding, which launched the ESRF's Foundation Phase in December 1985, was signed on the French side by Curien, who had become minister of research and technology. Three years later, on 16 December 1988, the ESRF convention was signed in Paris, and it was again Curien who represented the French government.

Despite his many commitments, Curien never lost contact with the ESRF. In November 2004 he paid a visit and expressed his admiration for the diversity and quality of the research carried out at the facility.

He received many honours, but Curien was a man of considerable warmth and simplicity. He will be remembered at the ESRF as a distinguished scientist and good friend. ●



● ESRF supporter. Scientist Jean Susini talks with Hubert Curien at the ESRF last year. Curien played a key part in the ESRF's history.

## Interview



**“It’s not difficult to recruit outstanding scientists these days. We get excellent candidates from all over the world.”**

**Ice breaker.** Elizabeth Moulin puts candidates at their ease to find out who they really are.

## ELIZABETH MOULIN: PERSONALITY ASSESSOR

**E**verybody knows the tension of being selected for a job interview: having to prove what you can do and convince a panel that you are the one that should get the job is not an easy task.

At the ESRF, candidates are lucky to bump into her at their arrival. Her welcoming smile breaks the ice immediately and makes them feel like talking. She is the first person who interviews them when they get to the ESRF. In about an hour she tries to find out about their personality – who they are. She is one of the two heads of recruitment, Elizabeth Moulin.

### **What do you need to work at the ESRF?**

Most of the people we recruit are sci-

entists, so in my interview I basically look for motivation, autonomy, initiative, maturity and team spirit. It is important that the future employee fits well into the team that s/he’s supposed to be integrating into. Then there’s the scientific or technical knowledge, which is something that’s evaluated by the rest of the recruitment panel.

### **Do you manage to find all of these qualities?**

It is not difficult to recruit outstanding scientists these days. We get excellent candidates from all over the world. We tend to have more problems in recruiting PhD students and foreigners in non-executive positions, such as technicians.

### **Does age matter in your assessment?**

Yes, normally PhD students are from 21 to 25 years old, postdocs are from 24 to 33 and scientists are from 30 up to 40 years old or so. We have to make sure that people who come out of the ESRF at the end of their contract can find a job elsewhere, and therefore age is an important factor. (I must confess I have a little note on my board with birth years and equivalent ages so that I can work out a candidate’s age immediately.)

### **And is gender an important factor?**

Not really. We encourage women to apply for a position as well as men, but we don’t implement any kind of “posi-



tive discrimination” in favour of women. The “gender equal opportunity” concept is working very well at the ESRF quite naturally.

### How do you deal with candidates of so many different nationalities?

Very often you can pretty much tell whether a candidate is from the south or the north of Europe by the way s/he says “hello” in the very first contact. In general, southern candidates need to speak and hear everything, whereas northern people are more structured and you can give them all of the information written down. However, scientists are open to the international environment.

### How important is your point of view in a recruitment process?

I can’t oppose the selection of a candidate, but I can let the panel know if I have strong objections. My role is to see what the panel needs and try to go for the best candidate. One could say that I enter through the back door, witness things, listen and then help interviewers to think who could be the best potential employee. Then I can also help them to figure out how they can supervise this person to bring the best out of him/her. When I started at the ESRF, in 1997, human resources were not really taken into consideration for different reasons. Now most group leaders listen to what we have to say.

### Do you think you ever get it wrong?

Yes, it certainly happens. There was a case of a Japanese scientist whom ID15 staff were very keen on selecting because he was an outstanding researcher. I exchanged some e-mails

with him and, when he came for the interview, I couldn’t communicate. He didn’t speak a word of English, but he could write it really well. I thought it would never work: he couldn’t communicate in any other language than Japanese, nor his wife and child, and he came from a completely different culture. ID15 staff insisted on the fact that he was the best candidate. They recruited him and it was, to my surprise, an absolute success.

### What attracts candidates to the ESRF?

The ESRF as an international centre of excellence is already very appealing. There is also the environment: some of the candidates already know Grenoble and they are attracted by the mountains surrounding the city – the perfect place for people who like sports and nature.

### Maybe they find it easy to integrate, but what about their partners?

Most of those whom we recruit are single. In the case where there’s a partner, that’s often a problem – today most partners have a career going before leaving everything to follow their spouse. Suddenly they find themselves in an unknown city, with an unknown culture and unknown language, and with no immediate career opportunity. It’s hard, and even harder if they have children. One of the tasks the social worker has is to help the employee and his/her family to find their mark in this new environment. We also work with a company that takes care of relocation for newcomers (housing, opening a bank account, dealing with different requests – phone, water – finding a doctor, etc).

## IN A HYPERACTIVE WORLD OF HER OWN

Her office is a good place to find out more about this half-American, half-French woman. Behind her desk there’s a board full of postcards from exotic places, such as the Great Barrier Reef. “Some candidates send me postcards when they go back home or on holidays, even if they didn’t get the job,” Moulin says. Maybe it’s her “internationality” that affords her the know-how to deal with



candidates with ease.

In her office, classical music reigns. “It relaxes me”, she says.

Music is her hobby: she plays piano and percussion, often with all of her large family, which makes a “mini orchestra” of six people. This active woman also dedicates part of her time to interesting pastimes such as African dancing and downhill skiing. In her list of amusements, there’s also space for cycling to work in the cold winter snow. All of this takes place when she’s not working as a teacher in different management schools in Grenoble. “I can do all of that because I share my position with another recruiter. I feel very lucky, since it’s rare that an executive position is part time.” Her mouse pad in her office shows one of the Second World War posters made to encourage women to work. The title reads like a motto for life: “We Can Do It!”

MC

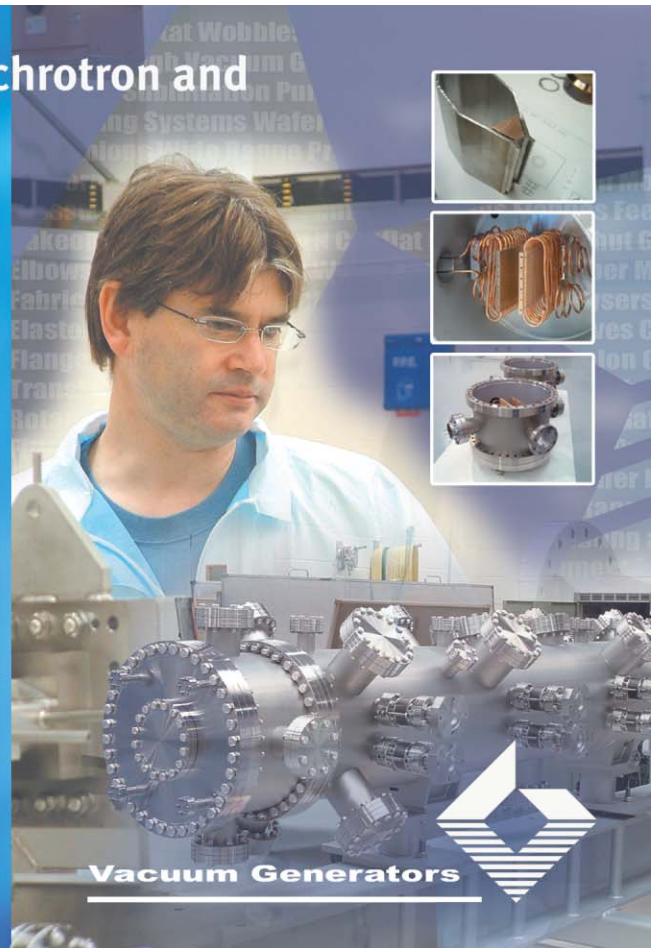
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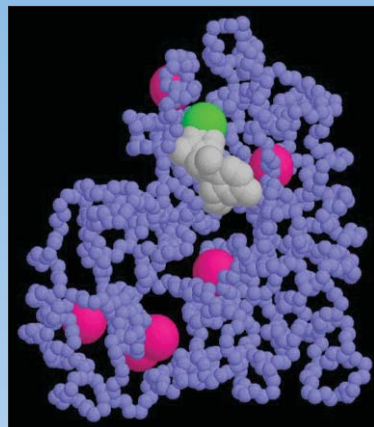


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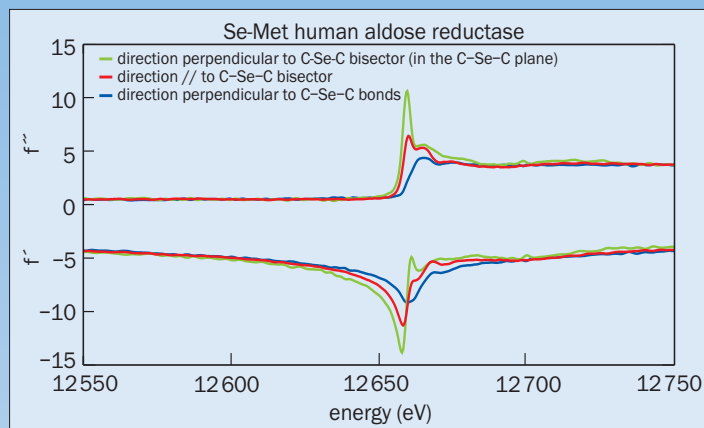


## Scientific highlights



**Figure 1.** Human aldose reductase comprising six Se atoms, one Br atom and 3200 non-hydrogen protein atoms.

**Figure 2.** Principal values of the resonant scattering tensors for Se in the selenomethionine residues.



## CRG BEAMLINES

### X-ray absorption, refraction and resonant scattering tensors in selenated protein crystals

G Bricogne,<sup>1</sup> S C Capelli,<sup>2</sup> G Evans,<sup>3,1</sup> A Mitschler,<sup>4</sup>  
P Pattison,<sup>5,7</sup> P Roversi,<sup>6,1</sup> M Schiltz<sup>7,1</sup>

1 Global Phasing Ltd, UK; 2 ESRF; 3 Diamond Project UK;  
4 Institut de Génétique et de Biologie Moléculaire et Cellulaire,  
Illkirch, France, 5 SNBL-ESRF; 6 University of Oxford, UK; 7 Ecole  
Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Atomic resonant scattering factors for an isolated atom are spherically symmetric. Chemical bonding in molecules and crystals can lower the symmetry and make atomic resonant scattering terms anisotropic. If the atoms and their bonds are oriented relative to the polarization of the incoming beam, the anisotropy of resonant scattering and absorption can be observed. Changes in some of the diffracted intensities can be seen as the orientation of the crystal is moved relative to the polarization of the incident synchrotron beam.

In addition to the effects on the diffracted intensities, linear dichroism can be observed. Dichroism manifests itself as anisotropy of absorption, and its effects can be seen both in polarized absorption and fluorescence spectra. The present study has been carried out on BM01A (Swiss Norwegian Beamline) on a selenated protein crystal (human aldose reductase) complexed with its cofactor NADP<sup>+</sup> and with the inhibitor IDD594 (figure 1). There is one molecule in the asymmetric unit, comprising 316 residues, of which there are six selenomethionines. The inhibitor contains a single Br atom that is covalently attached to a benzene ring.

Fluorescence spectra were recorded around the Se and Br K-edges for six different crystal orientations. Marked dichroism was observed in the polarized fluorescence spectra at both edges. In the monoclinic crystal system, the point group symmetry allows four independent elements for the absorption tensor and we have data in six orientations (figure 2).

Principal directions for the scattering tensor are (i) the direction perpendicular to the plane containing the C–Se–C bonds, (ii) the direction bisecting the C–Se–C angle and (iii) the mutually perpendicular direction. The resulting spectra of principal values of the Se scattering factors are plotted above, and we can therefore conclude that significant dichroism and anisotropic resonant scattering was observed in this selenated protein crystal.

These effects are therefore likely to occur in most standard MAD experiments, and they should be taken into account when designing the data-collection strategy and at the data-processing stage. In addition, the effects shown here can also be exploited, for example, by recording rotation data in several crystal orientations and extracting phase information from the observed intensity variations. ●

#### Reference

Bricogne *et al.* 2005 X-ray absorption, refraction and resonant scattering tensors in selenated protein crystals: implications for data collection strategies in macromolecular crystallography *J. App. Cryst.* **38** 168–182.

## CRG BEAMLINES

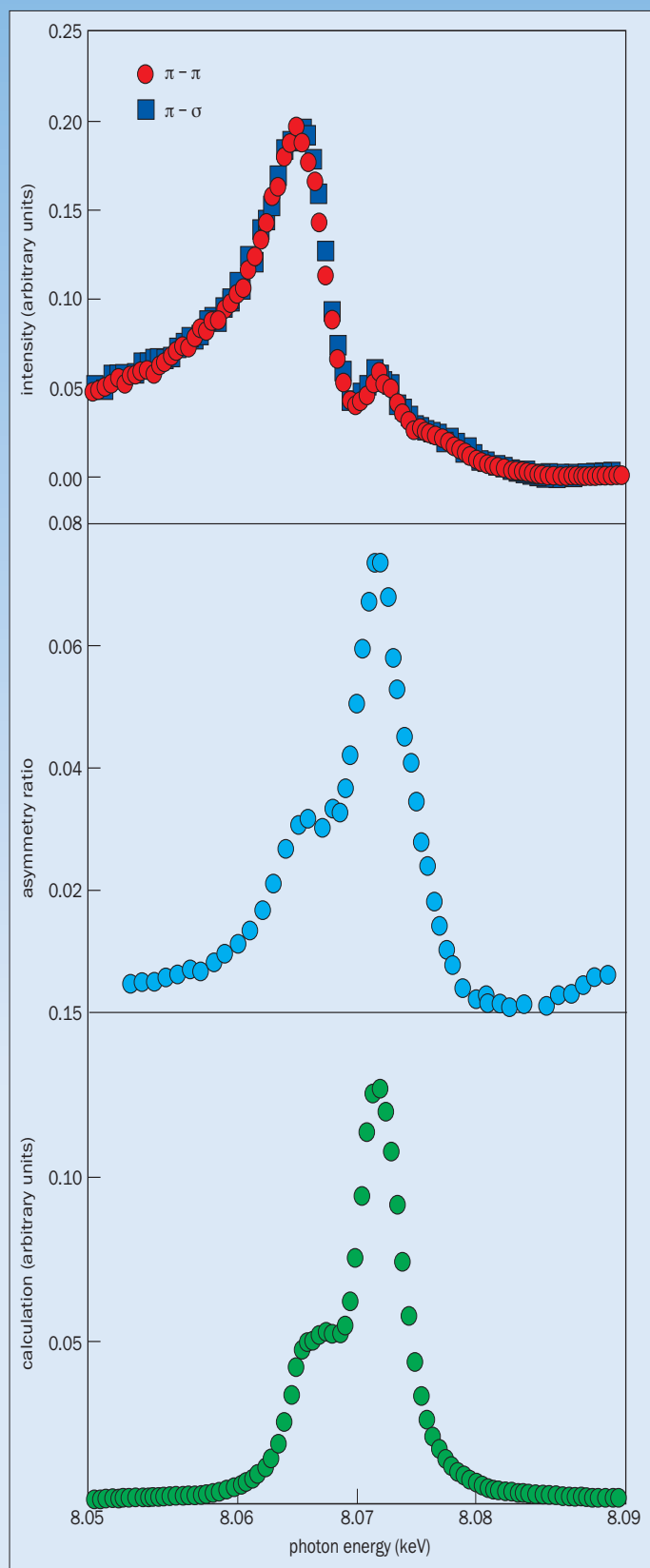
# Direct observation of giant d-band splitting in holmium

SD Brown,<sup>1</sup> L Bouchenoire,<sup>1</sup> P Strange,<sup>2</sup> P Thompson,<sup>1</sup> D Mannix<sup>1</sup>

1 ESRF XMAS beamline; 2 Keele University UK

The interpretation of rare-earth X-ray resonant magnetic scattering (XRMS) and X-ray magnetic circular dichroism (XMCD) at the L edges and the identification of dipolar (E1) and pre-edge quadrupolar (E2) features have been controversial subjects since the first experimental results were obtained. Previous studies of holmium have always led to purely quadrupolar assignment of the pre-edge peak. Ferromagnetic measurements were performed on XMAS, scattering horizontally from the (300) reflection through an angle of  $96.1^\circ$  at the  $L_3$  edge. Asymmetry ratios were obtained through reversal of a vertical magnetic field applied along the c axis, which are plotted in the middle panel of figure 3. From the angular terms in the XRMS cross-section, the quadrupole contribution is essentially zero in this configuration and we may thus conclusively assign both low- and high-energy peaks as dipole in origin, indicating a splitting of the d-band of 6.9 eV. In the purely antiferromagnetic phase, the (006- $\tau$ ) satellite was monitored while scattering through an angle of  $105.0^\circ$ . Polarization analysis was performed to isolate the  $\pi \rightarrow \pi$  and  $\pi \rightarrow \sigma$  scattering channels. The theoretical ratio of the dipole part of these two intensities is 2.52. The  $\pi \rightarrow \sigma$  intensity multiplied by 2.52 is plotted in the top panel of the figure along with the  $\pi \rightarrow \pi$  intensity (absorption corrected data are shown in the inset). The perfect superposition of these two spectra again demonstrates that both peaks are dipolar in origin. The theoretical method used to calculate the asymmetry ratio is a fully relativistic first-principles calculation based on standard time-dependent perturbation theory using the local spin density approximation to density functional theory with self-interaction corrections. The calculated asymmetry ratio is given in the lower panel.

We have shown that with XRMS it is possible virtually to turn off the quadrupolar signal. In its absence, a pre-edge resonance is observable of E1 origin. This result is in excellent agreement with the fully relativistic calculation and indicates a giant splitting of the d-band due to both exchange and large crystal field interactions.



**Figure 3.** Top: experimental antiferromagnetic  $\pi \rightarrow \pi$  and  $\pi \rightarrow \sigma$  intensity multiplied by 2.52. The superposition of these channels indicates the dipolar nature of both the low- and the high-energy peaks. (Inset: corrected absorption data.) Middle: experimental ferromagnetic asymmetry ratio. Here the theoretical quadrupole contribution is virtually zero, again indicating the dipole nature of both peaks. Bottom: the fully relativistic calculation convoluted with a 1.1 eV Gaussian representing the experimental resolution.



## CRG BEAMLINES

### Small-angle X-ray scattering of a supercritical electrolyte solution: the effect of density fluctuations on ion hydration

D Testemale,<sup>1,2</sup> M V Coulet,<sup>3</sup> J L Hazemann,<sup>1</sup> J P Simon,<sup>4</sup> F Bley,<sup>4</sup> O Geaymond,<sup>1</sup> R Argoud<sup>1</sup>

1 Laboratoire de Cristallographie CNRS, UPR5031, Grenoble; 2 SNBL/ESRF; 3 Laboratoire TECSEN, UMR6122, CNRS-Université Paul Cézanne, Marseille ; 4 Laboratoire de Thermodynamique et Physico-Chimie Métallurgiques, CNRS-INPG

Intermolecular interactions in aqueous solution under conditions of elevated temperature and pressure are related to the structure of the solvent and to the strength of the hydrogen bonding. Therefore, studying the structural and electronic evolution of solute particles with changing conditions of temperature and pressure is a way of obtaining information about the solvent itself. This research was carried out on BM02.

The aim of our studies is to understand the relation between physical properties and structural organization of liquids under conditions of elevated temperature and pressure, up to and beyond their critical point. These studies are possible thanks to a combination of the extremely bright and well focused X-ray beams at the ESRF with specially developed high-temperature and high-pressure cells. Synchrotron small-angle X-ray scattering measurements on water and zinc bromide ( $\text{ZnBr}_2$ ) aqueous solutions were carried out from ambient to supercritical conditions.

For both systems several isobars (285–600 bar) were followed beyond the critical isochore. The data were then

analysed through an Ornstein–Zernike formalism in terms of correlation length and null angle structure factor. The results for pure water are in agreement with previously published values. Solutions of different electrolyte concentrations were studied. In each case the values of the correlation length and null angle structure factor are larger than those of pure water. This effect is more pronounced for higher concentrations and/or pressures that are closer to the critical point of pure water. This is in agreement with the shift of the critical point determined in the literature for NaCl solutions.

Comparing these results to previous X-ray absorption measurements carried out on identical samples we propose the following two-step sequence for ionic hydration up to supercritical conditions: 1) from ambient to about 300 °C, an increase of ion pairing and formation of multi-ionic complexes that can be correlated to the decrease of the dielectric constant, 2) an enhancement of the local solvation shell of ions due to the onset of the thermal density fluctuations at high temperature, leading to a screening effect between ions and inhibiting the ion-pairing processes. ●

#### Reference

Testemale *et al.* 2004 Structural and electronic evolution of the  $\text{As}(\text{OH})_3$  molecule in high temperature aqueous solutions: an X-ray absorption investigation *J. Chem. Phys.* **121** 8973.

## OPTICS GROUP

### Smoothing of tungsten films by ion polishing

L Peverini, E Ziegler ESRF

We have investigated the evolution of a tungsten layer surface exposed to a 1 keV Ar ion beam at an incidence angle of 10° with respect to the surface plane. The ion-erosion process was followed *in situ* and in real-time via grazing incidence X-ray scattering. The time-dependent roughening of the film was then analysed and three main dynamic regimes were identified: surface smoothing, ripple formation and coarsening.

During surface smoothing the RMS roughness was reduced from 0.2 nm down to 0.17 nm. The data indicate that the tungsten film should not be exposed for a time longer than 200 s in order to avoid a gradual increase in the roughness. The possibility of surface smoothing is eventually expected to play a key role in the development of highly polished reflective optics, in particular for the synthesis of multi-layer coatings and for the final correction of figured X-ray mirrors. ●

#### Reference

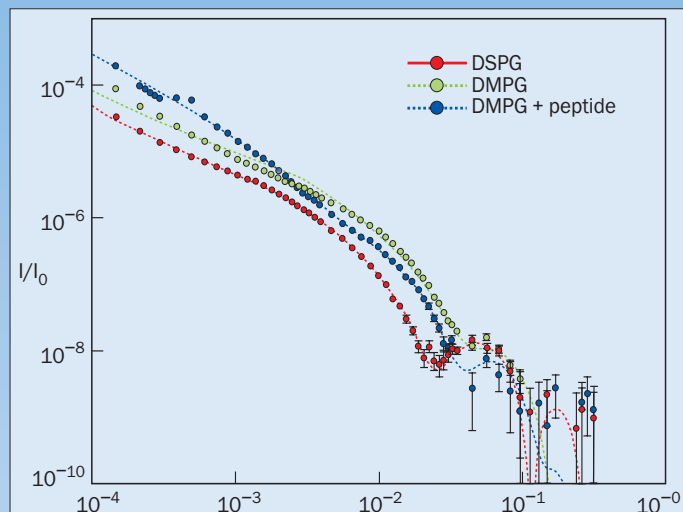
L Peverini *et al.* (in press) Roughness conformity during tungsten film growth: an in-situ synchrotron X-ray scattering study *Phys. Rev. B*.

## SOFT CONDENSED MATTER GROUP

## New possibilities at ID10B: high energy for surface studies at liquid/liquid interfaces

O Konovalov,<sup>1</sup> E Saint-Martin,<sup>1</sup> J Daillant,<sup>2</sup> D Luzet,<sup>2</sup>  
V Padmanabhan<sup>2</sup>  
1 ESRF; 2 CEA, Saclay-SCM/LIONS, France

The recent upgrade of the ID10B optics expands the available energy range to 22 keV. This allows studying buried interfaces (solid/liquid and in particular liquid/liquid), which play an important role in many biological processes. Experiments on such interfaces require a high energy as the X-ray beam is absorbed on its way through the liquid. For the first time at the ESRF, this has allowed us to apply all possible surface scattering techniques to an organic monolayer formed at the interface of liquid hexadecane and water. The X-ray beam travelled through 70 mm of hexadecane. In this way the specular reflectivity signal, off-specular and diffuse scattering spectra were obtained. Figure 4



**Figure 4.** Diffuse scattering (symbols) and the best fit (lines) measured at a grazing angle below the critical angle of total reflection at a hexadecane/water interface for DSPC, DMPG and DMPG in the presence of an antimicrobial peptide PGLa.

shows diffuse scattering (symbols) and the best fit (lines) measured at a grazing angle below the critical angle of total reflection at a hexadecane/water interface for 1) a monolayer of phospholipids distearoyl-phosphatidylcholine (DSPC), 2) a monolayer of phospholipids dimiristoyl-phosphatidylglycerol (DMPG) and 3) a monolayer of DMPG in the presence of an antimicrobial peptide, peptidyl-glycyl-leucine-carboxamide (PGLa).

From these data the vertical electron density profile of the film and its elastic constants were obtained. The bending rigidity of the films expressed in the units of  $K_B T$  is 40 for DSPC, 30 for DMPG and 10 for DMPG with peptides. The difference in rigidity between DSPC and DMPG can be explained by the difference in length of the aliphatic chains. The first molecule has 18 hydrocarbon groups while the second has only 14. This difference is seen in the change of van der Waals' interaction between molecules and consequently also in the elastic constants. Our results demonstrate that the addition of peptides to the negatively charged membrane of DMPG reduces the rigidity of the film.

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# HIGH RESOLUTION AND RESONANCE SCATTERING GROUP

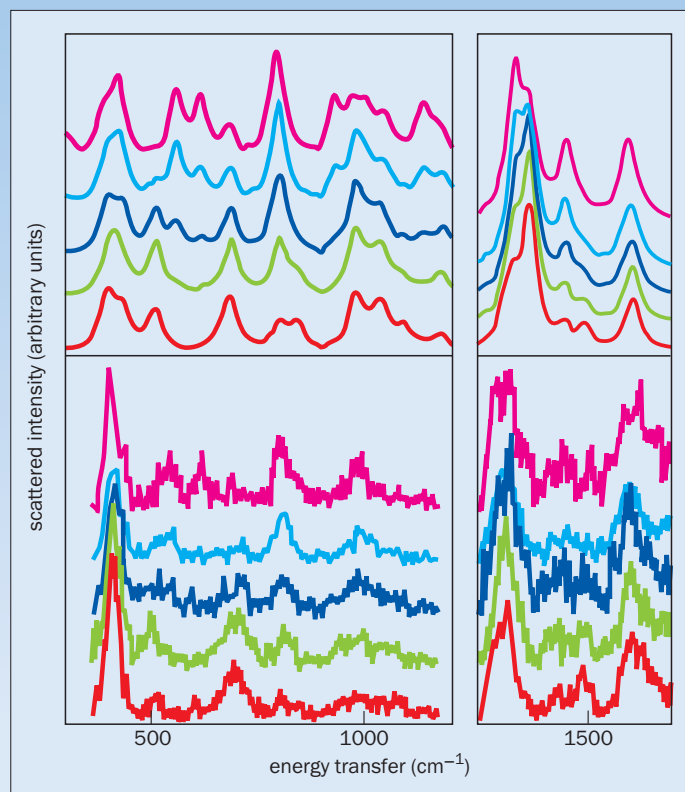
## Probing vibrational excitations in molecular crystals by inelastic X-ray scattering: from neutrons to X-rays

M Plazanet,<sup>1</sup> A Beraud,<sup>2</sup> M Johnson,<sup>1</sup> M Krisch,<sup>2</sup> H P Trommsdorff<sup>3</sup>

1 ILL; 2 ESRF; 3 Laboratoire de Spectrométrie physique, Université J Fourier Grenoble/CNRS

Inelastic X-ray scattering spectra of single crystals of benzoic acid have been recorded as a function of the momentum transfer vector,  $Q$ , in the 300–1800  $\text{cm}^{-1}$  frequency range (figure 5). These first measurements made in a molecular crystal are confronted with calculations, using density functional theory. Despite the limited signal-to-noise ratio, all spectral features and their  $Q$ -vector dependence are well reproduced. Considerable improvements can be envisaged by relaxing the  $Q$ -resolution and, most important, by increasing the solid angle of detection of the scattered photons. These developments are within reach and will render IXS a viable technique for the study of molecular vibrational modes, especially in the frequency range above 1000  $\text{cm}^{-1}$ , where neutron methods are limited in terms of energy resolution. This research was carried out on ID28.

Figure 5. Calculated (top) and experimental (bottom) IXS spectra of single crystals of benzoic acid for  $Q=(0, 3+x, 0)$ . Left:  $x=-0.2, 0, 0.19, 0.38, 0.58$  (bottom to top). Right:  $x=-0.14, 0.06, 0.25, 0.44, 0.64$ .



## MATERIALS SCIENCE GROUP

### Simultaneous tomography and diffraction analysis of creep damage

A Pyzalla,<sup>1</sup> B Camin,<sup>2</sup> T Buslaps,<sup>3</sup> M di Michiel,<sup>3</sup>  
H Kaminski,<sup>1</sup> A Kottar,<sup>1</sup> A Pernack,<sup>2</sup> W Reimers<sup>2</sup>

1 Technical University Wien; 2 Technical University Berlin; 3 ESRF

Creep damage by void nucleation and growth controls the lifetime of components subjected to loading at high temperatures. Combined tomography and diffraction experiments using high-energy synchrotron radiation on ID15 are used to follow *in situ* void growth and microstructure development in bulk samples. The results reveal that void growth versus time follows an exponential growth law and that the formation of large void volumes coincides with texture evo-

lution and a steady state in the development of dislocation density. Creep damage during a large proportion of sample creep life is homogeneous before damage localization occurs, which leads to rapid failure. The *in situ* determination of void evolution in bulk samples opens up new ways toward the assessment of creep damage in metallic materials and subsequently towards lifetime predictions of samples and components subject to high-temperature loading.

#### Reference

Pyzalla *et al.* 2005 Simultaneous tomography and diffraction analysis of creep damage *Science* **308** 92–95.

## Technical article

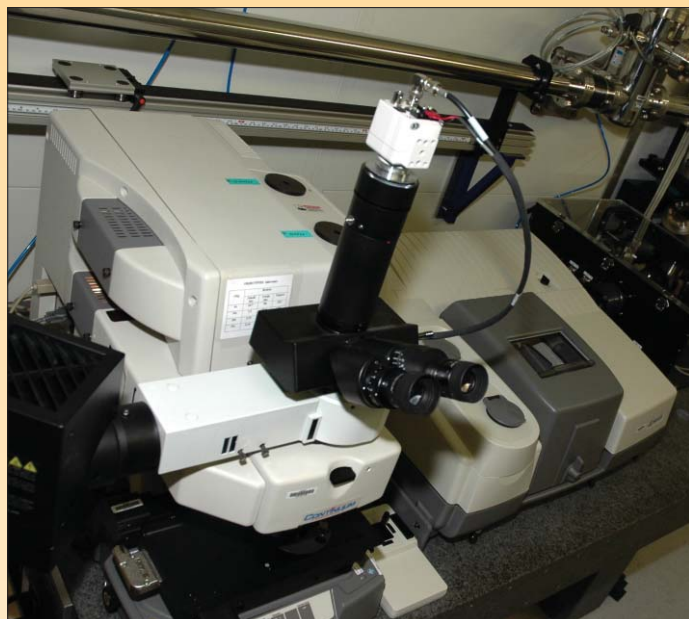


Figure 1: Overview of the endline coupling optics, spectrometer, mirror box and microscope of the infrared microscopy end-station.

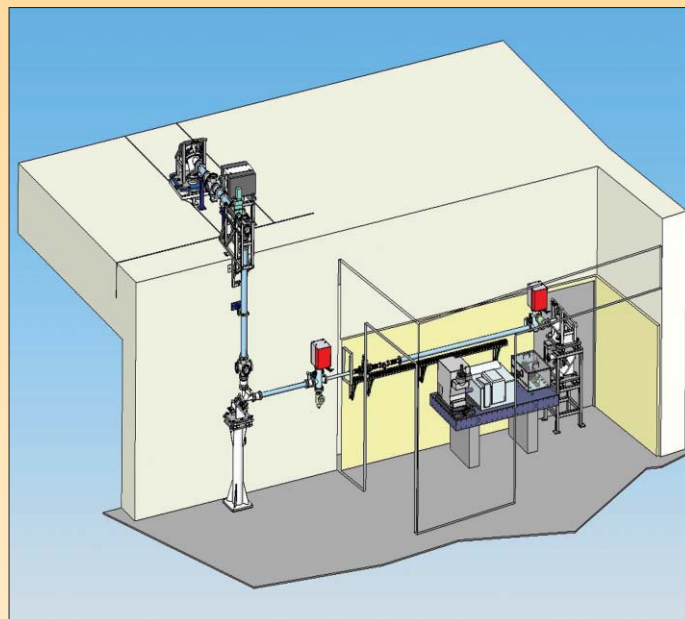


Figure 2: Schematic diagram of the infrared lab with the transfer line from the M3 mirror on the roof slab to the microscope lab.

## WHY INFRARED SPECTROMICROSCOPY AT THE ESRF?

J Susini, K Scheidt and M Cotte, ESRF; P Dumas, F Polack and O Chubar, Soleil

Infrared microspectroscopy is now a widespread analytical technique that combines the spatial resolution of a microscope with the high chemical selectivity of infrared (IR) spectroscopy. In particular the mid-IR spectral range 2.5–25  $\mu\text{m}$  (4000–400  $\text{cm}^{-1}$ ) is very informative because most of the organic and inorganic molecular groups have vibrational energies (“fingerprint modes”) in this spectral domain. The possibility of mapping particular functional groups’ concentrations in a homogeneous or heterogeneous sample in various states (gas, liquid or solid) with a few microns lateral resolution has made this technique very attractive in material characterization, and chemical and biological analyses.

Infrared microspectroscopy became even more powerful with the advent of rapid scan Fourier transform infrared (FTIR) spectrometers in the 1980s. However, the requirements of the IR sources, detectors and transfer optics are becoming more stringent. As with other microscopes, the performance of IR spectromicroscopes is limited by the source brightness. Despite a lower brightness compared with IR lasers, synchrotron radiation provides a broad spectral emission and wavelength tunability, as such required by

advanced commercial FTIR microscopes. In addition, the spatial resolution is no longer controlled by the geometrical aperture size but rather by the numerical aperture of the optical system and the wavelength of the light. Therefore the spot size is set to diffraction limit (a few microns).

The advantages of synchrotron IR radiation for microspectroscopy have already been demonstrated and exploited in most of the synchrotron facilities. The development of a similar instrument at the ESRF was driven by two major considerations:

- The number of IR photons, emitted either from a dipole edge or from a constant magnetic field, is essentially determined by the electron current in the storage ring. Therefore, despite being a high-energy machine, the ESRF is a good IR source as long as the appropriate collection geometry is fulfilled. Computations (using a Synchrotron Radiation Workshop (SRW) code developed at the ESRF) show that one can expect a photon flux compatible with a competitive scientific programme. Most important is that the infrared spectral region is known to be very sensitive to the synchrotron source stability and consequently this project should benefit from the ESRF machine performance. First performance studies confirm this expectation.
- The development of microanalysis and microspectroscopy



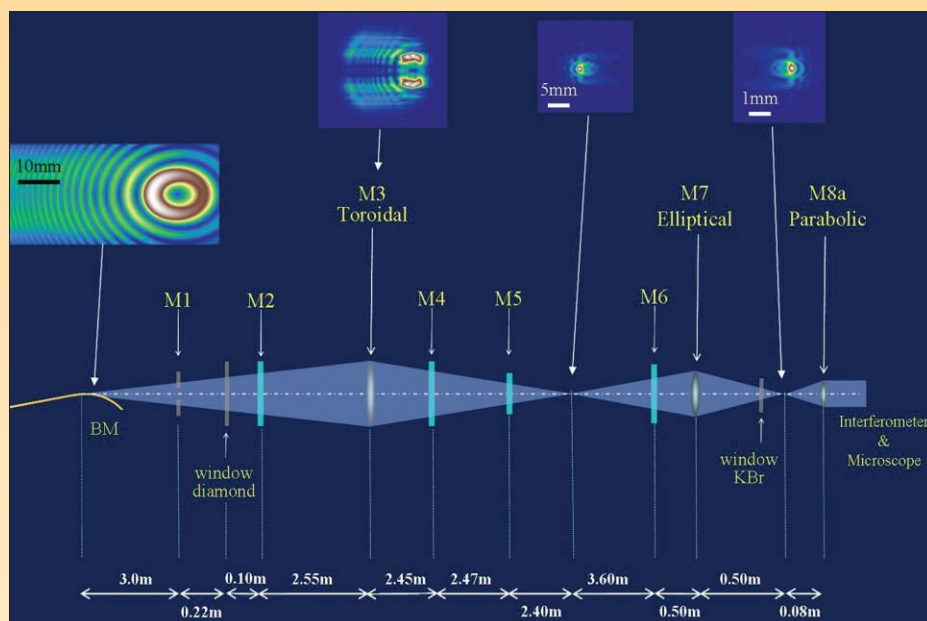


Figure 3: Optical layout and beam profile for a wavelength of  $10\ \mu\text{m}$  calculated using SRW.

methods, combining spatial and spectral resolutions, has already attracted several very active user communities at the ESRF. It is worth noting that the different scientific communities that are interested in performing microanalysis, using either IR or X-ray photons, are essentially the same. Most of the scientific cases require a multimodal approach, consisting of a coupling of techniques providing chemical as well as structural information.

This project aimed to build a competitive IR microscopy end-station (in terms of brightness and source stability) in order to set the first X-ray/IR analysis platform, which would constitute a potential and unique synchrotron-based microcharacterization facility (figures 1 and 2). Such a project has resulted from a close collaboration between the Machine Division and the Experiments Division.

### It's all done with mirrors

The extraction mirror was one of the most critical technical challenges. A new dipole chamber with enlarged vertical opening had to be installed in cell 22. Edge geometry (i.e. the edge radiation emitted from the short, straight section – focusing electron lenses – upstream of the bending magnet) was preferred. The extraction mirror located at 3.2 m from the dipole entrance is a flat uncooled aluminium mirror with a horizontal slot. This 5 mm slotted-aperture lets the energetic part of the synchrotron light go through for absorption 2.5 m farther down. The mirror assembly is vertically movable, and by the use of thermoprobes, located

on its backside and separated by 2.5 mm, the slot is kept vertically centred on the heart of the X-ray beam in a slow feedback loop. The edge radiation from both upstream and downstream dipoles as well as constant field radiation is collected and transferred to the spectrometer and microscope via a series of nine mirrors. The optical concept aimed at reaching the best matching of the IR beam divergence with the microscope Schwarzschild lens aperture.

This strategy was optimized by modelling the entire line using SRW (figure 3). Preliminary performance tests confirmed that the beamline is free of

wavefront distortion and vibrations, thus preserving the brightness of the ESRF source. High intensity at the detector stage is obtained, even for aperture sizes as low as  $3 \times 3\ \mu\text{m}^2$  (in a true confocal collection geometry). The Thermo Nicolet Nexus IR bench is associated with an infrared Thermo Continuum microscope. The latter has several features customized for various synchrotron applications: visualization of the sample even while acquiring data; infinity-corrected optics, which allow additional optical systems to be inserted, such as visual and infrared polarizers; Nomarski differential interference contrast optics; and UV fluorescence. These features are useful in identifying a given region of interest in the sample. A specific sample holder with fiducial indexation has been developed to allow the sample to be transferred and realigned from the IR microscope to the X-ray microscope.

Most of the scientific activities of the X-ray microanalysis beamlines, ID21 and ID22, are method oriented. The development of this IR microscopy facility is expected to boost several programmes by enhancing our microcharacterization capability. Several ongoing programmes on archaeometry, bone structure/chemistry, microirradiation at the cell level, plaques in brain tissues, sulphur microspectroscopy in volcanic microinclusions, and microstructure in electronic devices will no doubt benefit from the instrument.

• This project has benefited from the involvement and active participation of M Salomé, D Eichert, S Bohic, C Hirschmugl, R Baker, E Gagliardini, B Plan and P Duru.

## User's view



"You'll never be a chemist!" Serena Margadonna receives the Young Scientist Award from Philip Evans of the MRC Laboratory of Molecular Biology, Cambridge, UK, thus proving her chemistry teacher wrong.

**"The ESRF is an institution of excellence where world-leading scientific research is constantly performed. I am tremendously proud that my work has been considered part of this excellence."**

## SERENA MARGADONNA – WINNER OF THE 2005 ESRF YOUNG SCIENTIST AWARD

**W**hen she was in high school her chemistry teacher told her that she would never be able to be a chemist. Instead of discouraging her, however, this provoked the opposite reaction, and Serena Margadonna was from then on determined to give science an important role in her life. Today, at 32, she is a researcher who is thirsty for knowledge and a lecturer in chemistry at the University of Edinburgh.

The synchrotron came into Margadonna's life when she had barely begun her PhD at the University of Sussex. She has always used powder diffraction to perform her experiments and often visits ID31, BM01 or ID24. The main thrust of her research has been on multifunctional molecular materials, especially fullerides. Her work at the ESRF has been recognized in the Young Scientist Award, which the Users' Organisation presented to her last February.

### What does the YSA represent for you?

It is a great honour and a big achievement. The ESRF is an institution of excellence where world-leading scientific research is constantly performed. I am tremendously proud that my work has been considered part of this excellence.

### How important is a synchrotron in your work?

Access to the ESRF and synchrotron radiation has been of fundamental importance for the development of my work because it has allowed me to study the structural properties of highly disordered materials in unprecedented detail and understand the complex structure-property relationships of high correlated electron systems.

### What's new in your field?

My research focuses on molecular mat-

erials and the effect of external stimuli, such as temperature, pressure and light illumination, on their properties. I think there is a whole world of interesting materials and effects out there. Every year there are two or three new discoveries related to my research, and they open up new approaches. I also try to broaden my expertise, so I've joined the Centre for Science at Extreme Conditions in the UK. This brings together expertise and equipment to study materials at extremes of pressure, extremes of temperature and in electromagnetic fields. It serves to unite researchers across a wide range of disciplines – chemistry, physics, earth sciences, engineering, materials science and biology.

**You have just started a new period in your career by taking a permanent position as lecturer at**



## Edinburgh University. Is teaching tougher than doing research?

Lecturing is tough and demanding, and you tend to spend a great deal of time thinking how to explain the subject. However, at present, because of my concurrent Royal Society Dorothy Hodgkin Research Fellowship, I don't give too many lectures and I can dedicate most of my time to research. And it is a permanent position, which gives me a lot of stability.

## So, you have no intention of going back to Italy in the short term?

Life in the UK is different from that in Italy and it rains a lot in Edinburgh. However, in the UK I am free to do my research the way I want. Despite my age, I am building my own research group, which would be something quite unlikely to happen in Italy at this stage.

## How do you see the responsibility of leading a group?

Leading a group is certainly a big challenge. However, for the last few years I have been taking care of all aspects of an experiment – from sample preparation to writing papers. With the team, which will include two or more people, I'll be relieved of some of these tasks and I will therefore be able to concentrate more on strategic issues in research.

## Have you encountered any difficulties in your work as a scientist as a result of being a woman?

I haven't experienced any discrimination and I do not think that women are special. Scientists behave professionally in the same way, irrespective of gender. I think it will be tough when I have a family, because research is not

the best job when you have a partner and children. I believe there is a bond between mother and child, and it is necessary for the mother to stay constantly with the baby at least in the first years of its life. Nevertheless, family and career can be compatible when you have a group that can keep things going while you are away on maternity leave.

## What would you suggest as a solution to this problem then?

I would suggest that government bodies provide special postdoctoral positions that would replace pregnant women who are just about to leave to give birth. This would help the future mother by letting her be absent from her job for a while and then quickly catch up on her return without losing her momentum.

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## ESRF Newsletter December issue

The international scientific community expects ever-higher performance and efficiency from equipment for their research sites. If you want to remain at the vanguard of instrument and infrastructure supply for synchrotron radiation, it is imperative for your company to reinforce its identity to this community. *ESRF Newsletter* will assist in this.



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## Visiting a beamline



**Automation is key.** From left: David Flot, scientist ID23-2; Joanne McCarthy, BLOM; Matias Guijarro, BLISS; Didier Nurizzo, scientist ID23-1; Vicente Rey, BLISS. Absent are Thierry Giraud, Mario Lentini, Gordon Leonard, Trevor Mairs, Sean McSweeney, Ed Mitchell, John Surr.

## MACROMOLECULAR CRYSTALLOGRAPHY GROUP HAS NEW BABY

The team responsible for the new ID23 beamline have focused on automating as many of the instruments' features as possible to make experiments easier.

When you enter the control cabin the flat screens on the wall as well as the new furniture indicate that the beamline is brand new. ID23 (Gemini) is the most recent beamline of the Macromolecular Crystallography (MX) Group and it was built to absorb the increasing demands for protein crystallography beamtime. The most automated beamline of the ESRF is already open to users in one station, and users will be able to apply for beamtime on the second station for the September round.

The key feature of ID23 is "automation". "We've tried to conceive an automated beamline from the start," said Didier Nurizzo, the scientist in charge of the first station. The teamwork of the BLISS (Beamline Instrumental Software Support) group, the Technical Beamline Support group and the scientists from the ESRF and the European Molecular Biology Laboratory (EMBL) has made it possible to build a beamline with many automated features: the optical elements are all independent and can be aligned and prealigned automatically; and a sample changer has recently been installed. The beamline also has a minidiffractometer, which has a very high precision of rotation allowing small samples to be used. It will also have a new very-large-area CCD-based detector, which is essential for optimizing data collection from certain valuable samples. All of these features will help the users to carry out their experiments in an easy and

reliable way. At the moment the MX group has, on average, six user groups per week per beamline, so automation is extremely important: "If you come only for one day, you can't spend your time setting things up," explained David Flot, the scientist in charge of the second station.

Owing to the automation, ID23 is a beamline with only two scientists — one per station. Technicians and support groups are shared with the rest of the MX beamlines, which act together. This has been enough to conceive and build ID23-1 in two years' time. ID23-2, which may provide a focused beam down to 5 µm in diameter to allow protein microcrystals to be probed, will be the first microfocusing beamline dedicated fully to macromolecular crystallography.

Every Monday the ID23 team meets to discuss the developments on the beamline. In the first days of ID23, they had a celebration every time an important step forward was made on the beamline. The first user on ID23-1 was also a good excuse for a party. Today, users come to this first station so often that they are no longer an "event", and fewer elements are being installed on the beamline, even if it is still being developed. Nevertheless, soon the first users on ID23-2 will give the team reason to drink a toast again to this high-throughput automated beamline.

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## CARL-IVAR BRANDEN BUILDING IS ALMOST READY

The ESRF beamline ID23 is associated with the scientific programme of the Partnership for Structural Biology (PSB). The PSB is set to become a structural biology centre unique in the world. The construction of a new laboratory complex will be completed during the summer, and the scientists will have moved in by the end of the year.





## Gallery of events



Herculean effort. Postgrads, postdocs and staff at HERCULES 2005 tear themselves away from studying synchrotron and neutron radiation.

## COURSE AIMS TO MAKE KNOWLEDGE IN X-RAY AND NEUTRON TECHNIQUES STRONGER

HERCULES 2005 celebrates its 15th anniversary and its 1000th participant, it confirms EC recognition and it will add new specialized courses.

**H**ercules is the Roman name for a hero in Greek mythology who was particularly noted for his strength and courage. HERCULES (Higher European Research Course for Users of Large Experimental Systems) is also a European training course on the use of large instruments, which, one could say, strengthens its young attendants' knowledge of synchrotron and neutron radiation. Last February this five-weeks event welcomed 77 scientists (mainly PhD students and postdocs) in Grenoble, and among them the 1000th participant in HERCULES.

The event is organized by the Université Joseph Fourier (UJF) and the Institut National Polytechnique de Grenoble, with the invaluable help and support of large partner synchrotron radiation and neutron facilities. This training programme will be extended over the next four years, thanks to the support of the European Commission 6th Framework Programme of Research and Development. Indeed, the pro-

ject presented by the HERCULES organizing team was ranked first above more than 370 other applications.

PhD students and postdoctoral scientists from 23 different countries participated in February and March to HERCULES 2005. They not only learned more about the use of synchrotron and neutron radiation for the study of condensed matter but also were able to feel the atmosphere associated with this type of research. "I was greatly inspired by the international atmosphere to continue with my own studies in a more creative way," explained one of the participants. "It opens your mind," added Pedro Fernández, from the Institute Laue Langevin (ILL).

### Practical participation

The training combines both theoretical and tutorial courses with practical lessons performed using synchrotron and neutron radiation state-of-the-art instruments. The practicals took place at the ILL and ESRF, as well as at Laboratoire Léon Brillouin in France and ELETTRA in Italy. They are always appreciated by the participants. "The part I enjoyed the most was the visits to the various beamlines and getting a

bit of a touch on the equipment. At the end of the day – and this is unique to the course – not everyone has an accelerator or reactor for in-house research,” said Plamen Stamenov from Trinity College in Dublin in Ireland. “There should be more tutorials/practical sessions,” said Roberta Poloni from the ESRF.

In addition to the now well established five-week “general” HERCULES course, each year the training will include three one-week HERCULES Specialized Courses (HSC). The ESRF is strongly involved in the organization of the HSCs, the scientist in charge of them being José Baruchel. The first HSC, in 2006, will be on structural genomics, synchrotron X-ray imaging and surfaces, interfaces and nanostructures. This will be followed, in 2007, by courses on magnetism, new approaches for biology, and cultural heritage.

“The aim of this HERCULES project is to create an international school on large instruments for condensed matter studies in Grenoble – a unique place in Europe because of the simultaneous presence of the ESRF and the ILL, and the huge scientific potential in the surrounding labs and universities,” said Jean-René Regnard, professor at the Université Joseph Fourier, a founder of HERCULES and its current director. •

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## HERCULES 2006

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**Neutron and synchrotron radiation for physics and chemistry of condensed matter**

Session B

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**HERCULES**

**CNRS – Maison des Magistères**  
**BP 166**

**38042 Grenoble Cedex 9**

**Tel: +33 (0)4 76 88 79 86**

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## THE ESRF CELEBRATES ITS 15TH USERS' MEETING

The 15th ESRF Users' Meeting in February focused on the Long-Term Strategy, which defines the goals of the ESRF for the next 10–20 years but there was also time to celebrate the first decade of users at the ESRF.

**A**t the 2004 ESRF Users' Meeting, delegates were asked for their views on the future development of the ESRF. They said that they wished for more beamtime and that it was important to retain the stability and reliability of the machine.

Within the Long-Term Strategy, the ESRF is considering how to achieve these aims. Some possibilities were presented at the 2005 ESRF Users' Meeting in February, which attracted around 300 scientists from around the world. Ideas included increasing the number of beamlines (~10 more) to provide the users with more beamtime; increasing the size of the Experimental Hall; and opening the ESRF up to new scientific communities.



**The future looks bright.** Chairman of the Users' Organisation, Marco Grioni, opens one of the umbrellas made as gifts for the celebration of the first decade of ESRF users.

The event also looked back a decade, when users began coming to the ESRF. In this context, Massimo Altarelli, former director of research and now senior scientific director of the Italian synchrotron ELETTRA, gave a speech.

The ESRF director general, Bill Stirling, pointed out that the number of scientific proposals has increased from 312 for six months in 1994 to 901 in the last six months of 2004, which clearly illustrates the significant increase in interest of the users.

The meeting also included a fascinating plenary talk by Fotis Kafatos, director of the EMBL until May, entitled “Life science in the early 21st century: an endless frontier”.

An update on the status of the building that will host the



Partnership for Structural Biology (PSB) was presented by Sine Larsen. The laboratory building will be ready by October 2005. It has been named after a former research director at the ESRF, Carl-Ivar Brändén, who played an important role in the development of structural biology there. The PSB combines the scientific expertise of different institutes to determine the structure of proteins and other macromolecules that are key to biological processes.

Currently there are discussions about creating a partnership for soft condensed matter and another one for materials science. These would need new facilities. There is

also a new project with the ILL and the EMBL to remodel the site entrance. This would be on the Avenue des Martyrs and the site would be equipped with a visitors centre, a bigger guest house, a restaurant, an auditorium for 400–500 people and other buildings for new scientific partnerships.

With all of these challenging goals, the ESRF is an even more tempting institute for countries to join. Discussions are taking place with Slovakia, Ireland, Greece and Baltic countries. Poland became a scientific associate in 2004, bringing to 18 the number of countries involved. ●

MC

## Satellite workshop: Synchrotron radiation in art and archaeology

Over recent years, many experiments (some pioneering) have been conducted at the ESRF on cultural heritage materials. This has been possible thanks to fruitful collaborations between synchrotron radiation scientists, museums, and archaeology and restoration institutes. Synchrotron radiation can provide powerful and complementary ways of obtaining greater insight into our physical and cultural past, so there is an increasing demand for access to synchrotron-radiation-based techniques, such as X-ray imaging, X-ray diffraction, X-ray absorption, X-ray fluorescence and infrared spectroscopy.

To bring together key members of the synchrotron-radiation community and experts in the disciplines of archaeology, archaeological science, art conservation and materials science, a joint ESRF–CNRS workshop took place

at the ESRF in February. Attended by 123 participants from 19 different countries, it explored a range of subjects relating to art and archaeology, from metals, ceramics and paintings to biology and molecular archaeology. It was also a great chance to discuss emerging synchrotron-radiation techniques as well as complementary methods, such as neutron scattering, and combined strategies.

The scientists highlighted that they should enhance communication with art curators and archaeologists, who often don't know about all of the research possibilities that synchrotron radiation offers. They also said that dedicated strategies and special devices to bring, prepare and measure samples at synchrotron radiation facilities are needed.

This is the third time that this community of scientists has met. The success of the event has made delegates foresee a new edition of the workshop in 2006. This would be organized by BESSY, the Technical University of Berlin and the Federal Institute for Materials Research and Testing. ●

ERIC DOORYHEE AND JEAN SUSINI

## Satellite workshop: New science with new detectors

The development and construction of new X-ray detectors will be key to the ESRF's Long-Term Strategy, so this workshop was organized for 9 and 10 February. The goal was to define scientific projects that could drive and steer such developments. The fact that there were more than 150 participants shows that X-ray detectors are increasingly in the focus of our users and scientists.

The satellite workshop began with overviews of the challenges at current and future X-ray sources, followed by a session on new detectors. Reviews of state-of-the-art detector technologies were given by some of the world leaders in the field. Particularly impressive is the progress made

in silicon drift diode detectors and in pixel detectors.

The second day was mainly dedicated to "new science", with a range of scientific fields from high-energy high-spatial resolution imaging to picosecond time-resolved scattering, from hard condensed matter to biological materials, and from fundamental physics to applied chemistry.

All of the presentations indicated that important scientific progress is possible with current sources and improved detectors. It was also clear that very often order-of-magnitude improvements can be achieved with current state-of-the-art detector technologies, provided that significant resources are dedicated to using these cutting-edge methods to build dedicated X-ray detector systems for synchrotron applications. ●

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using bi-metallic Atlas Flanges.

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