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ESRFnews

Number 49 March 2009

Making water crystal clear

Plans to upgrade the beamlines are taking shape

A chance discovery: a new fluorescent protein

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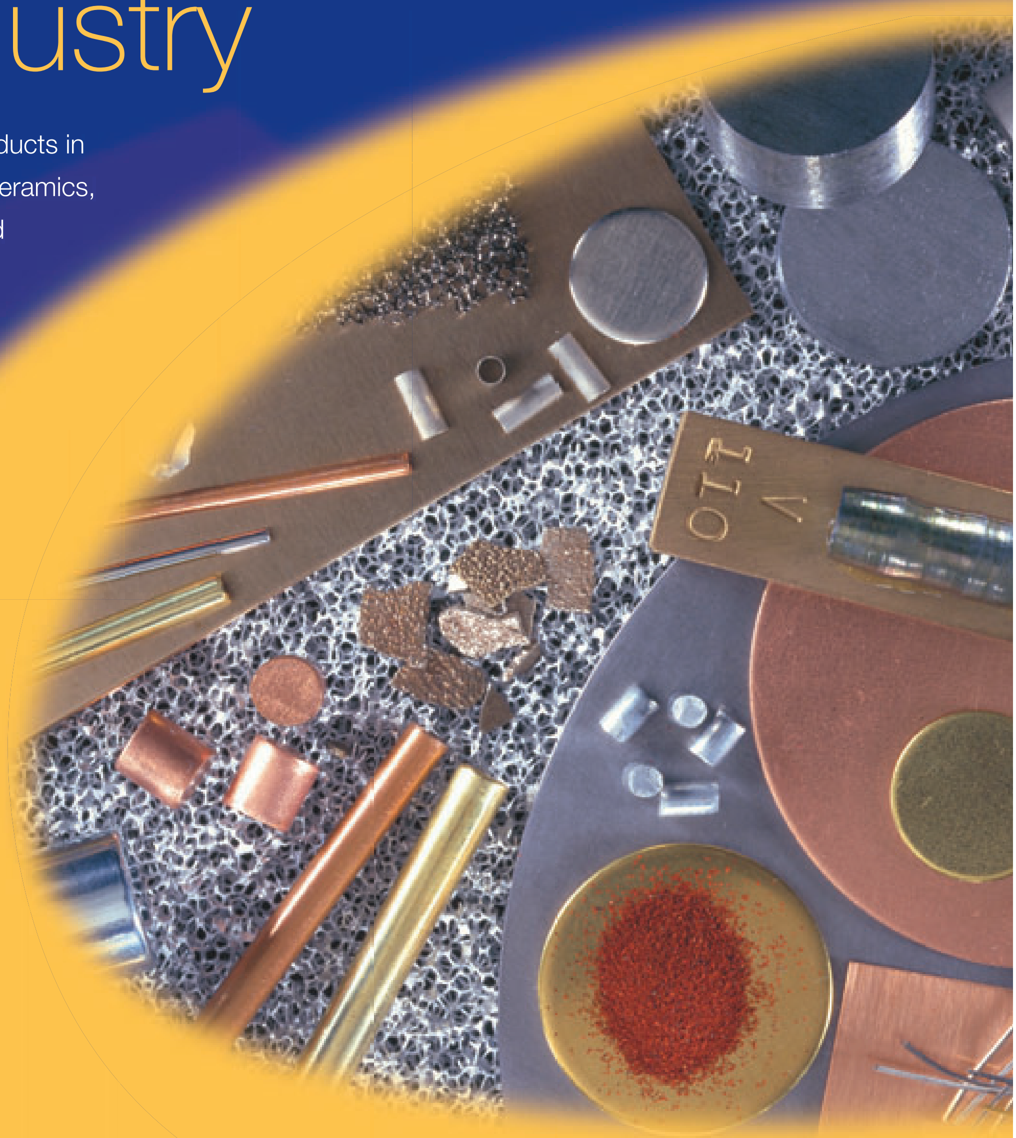

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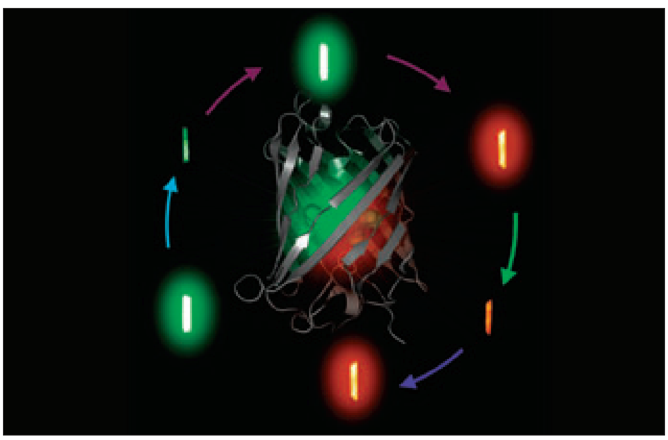
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On the cover: Synchrotrons are helping to make water clearer.

ESRFnews Number 49 March 2009

Photonic Science

Scientific Detector Systems

X-ray CCD detectors deliver down to 1.4 micron resolution

Photonic Science delivers a new generation of complete X-ray CCD systems for home lab and

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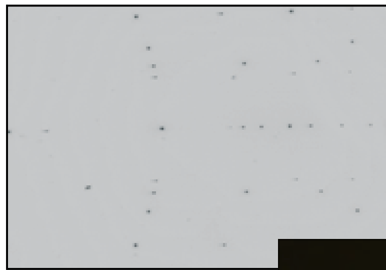
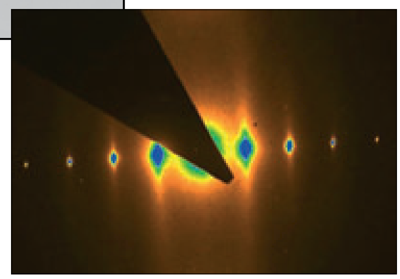


CuSi, 30 sec exposure 2µ beam size, bending magnet BM32 @ ESRF

Image courtesy X. Biquard, CEA/CNRS



colloidal goethite nanorods 50µ beam size, bending magnet BM26 @ ESRF

Image courtesy V. Petukhov, Utrecht University

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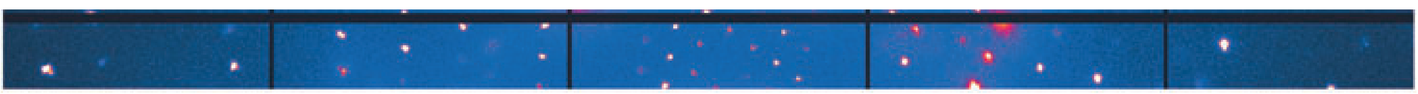

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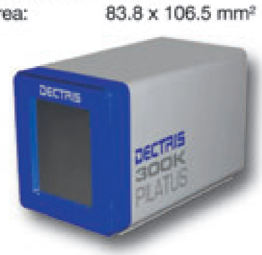

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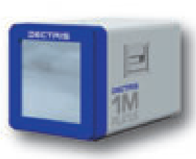

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Onwards and upwards

On behalf of all of the ESRF staff, I would like to wish all of our readers a wonderful 2009. All years are important, but, for the ESRF, 2009 will be particularly special.

The ESRF is officially starting a new and ambitious Upgrade Programme. At the end of 2008, the ESRF Council gave the green light for this challenging initiative, and, together with maintaining a maximum commitment to continued user operation and support, it will be our main priority in the years to come. This is a necessary step to keep the ESRF at the forefront of science and to foster research with synchrotron radiation, amid the rapidly evolving European and worldwide scenarios.

I have the honour, for the next five years, of leading the ESRF – an international laboratory to which I have belonged for many years with different responsibilities. I have watched the institute grow almost from the beginning. It has, in my opinion, set many examples for scientific research and collaboration in the field of synchrotron science, for its leadership in technical innovations and as an effective model of how to construct and operate a large international research infrastructure, in particular from an administrative and financial point of view. The ESRF celebrated its 20th anniversary in November 2008 and it is now preparing ambitiously for a bright future through the Upgrade Programme. I am thrilled to be a part of this adventure.

"The ESRF is preparing ambitiously for a bright future"

This second issue of *ESRFnews* in its new form takes as its scientific theme one of the best known, and yet still mysterious, substances: water. It is everywhere and it is considered to be one of the key elements required to foster life. It is necessary in our daily life, and it is a crucial element in both old and highly advanced industrial processes, as well as in agriculture. Water is also starting to become a cause for concern in sustainable development, and it is searched for in astronomy as an indication of life forms in outer space. However, it is also a molecule prompting many difficult scientific questions. With its tendency to form a fairly open structure with tetrahedral local ordering, it has, despite its chemical simplicity, one of the most complex phase diagrams showing a multitude of crystal phases (the exact origin of which is still being debated). In its liquid form it exhibits a density maximum with an origin that remains controversial. It shows glassy states with quite different densities, and many scientists are convinced that it could also display significantly different liquid phases.

The peculiarity of water is based on its subtle hydrogen bonding. This is, to a certain extent, at the core of all of its chemical and physical properties, such as its pH (i.e. the relative concentration of free OH^-/H_3O^+ ions, a macroscopic property that is intimately related to the chemical properties of water, strongly temperature dependent and of fundamental importance in biology). Understandably, water and its properties still pose extraordinary challenges in fundamental biology, chemistry and physics, but also in more applied sciences, such as environmental science, geology, glaciology, marine science and new industrial procedures. One of the most fundamental issues, which is often highlighted above all others, is the relationship between macroscopic properties and the local bonding and geometrical structure of water molecules. This correlation has been tackled for many years through studies carried out using neutrons and X-rays. In 2004, *Science* magazine defined the research on water as one of the breakthroughs of the year and referred to work carried out at different light sources. We dedicate this issue of *ESRFnews* to reviewing some of the research that uses the facility's beamlines.

A lot of good work is being carried out, but I am convinced that a better understanding of the many unique and delicate properties of the hydrogen bond is still one of the most challenging open questions in chemical physics, and this will have a tremendous impact on biology. I wish you all a good read and I would like to finish by citing Nobel Prize winner Linus Pauling: "The problem of the structure of liquid water has attracted much attention, but as yet no completely satisfactory solution to it has been found." (1980 *The Nature of the Chemical Bond* 3rd edn Cornell University Press p469).

Francesco Sette, ESRF director-general

Developers scoop a pair of awards

ESRF members have won two awards for developing technology of use to the scientific community. The BESSY Innovation on Synchrotron Radiation award was given to Vicente Rey Bakaikoa and Olof Svensson for "their decisive role and participation in the development of a customised software environment on the ESRF macromolecular crystallography (MX) beamlines", which has made it possible to screen crystals more quickly.

The winners made it clear that the prize recognizes the efforts of the Beam Line Instrumentation Software Support, the Scientific Software Groups, the MX Group, the Instrument Support Group and computing services at the ESRF, as well as external groups – notably the European Molecular Biology Laboratory.

A group of users, including ESRF scientist Peter Cloetens, won the Prix La Recherche 2008 in the Human Health section. This was awarded for the development of a technique that has enabled a multi-institution research team to create a 3D reconstruction of cerebral tissue with a volume of tens of cubic millimetres. The complex microvessel network feeds the normal development and function of the brain and the growth of brain tumours. Using an automatic numerical protocol that allows the quantitative analysis of such networks, it was found that both normal and tumoural vascular networks have a fractal structure. This suggests that the multiscale evolution of tumour growth dynamics may be a fruitful avenue for research.

New division will unite groups

This year the ESRF will create the Instrumentation and Support Development Division to offer a new support service, rationalizing instrumentation support by combining the skills of different groups. Groups stemming from the Experiments Division, computing services and technical services will be combined. New head Jean Susini, deputy head of the X-ray Imaging Group and responsible for beamlines ID21 and ID22, takes office on 1 March.

Symposium bids DG Bill Stirling farewell

Bill Stirling left his job as ESRF director-general at the end of 2008 but his colleagues didn't want him to leave without honoring him with a symposium on his research.

Entitled From Helium to Plutonium (with X-rays and Neutrons), the event went through the elements in the periodic table that Stirling has worked on: helium, uranium, etc. There was also a talk about the construction of the Xmas beamline, which was set up by Bill Stirling and Malcolm Cooper.

The presentations combined fundamental physics with anecdotes, and the speakers at the event were Stirling's friends and collaborators from Germany, the UK, the US, the ESRF and ILL.

Hydrogen reaches new pressure limits

Hydrogen is the simplest element possible, and yet details of the structure of its solid forms still remain a mystery. Merely solidifying hydrogen requires high pressures, and, once this elusive state has been attained, there are still challenges in taking measurements because samples scatter X-rays extremely weakly.

Researchers from the Centre à l'Energie Atomique and the high-pressure ID27 beamline at the ESRF have recently overcome these technical challenges to obtain diffraction images of a single crystal of hydrogen at the highest pressure yet achieved for these measurements – an impressive 190 GPa. For comparison, that's half of the pressure at the centre of the Earth. Previous spectroscopic measurements have shown that solid hydrogen can take three crystallographic forms: phase I, a regular close-packed lattice where the diatomic molecules are free to rotate; phase II, a more complicated structure with some local symmetry that varies in scale; and above 150 GPa, the as-yet-unknown phase III state.

The diffraction results from ID27 are currently being analysed and it is hoped that they will shed light on the structure of the elusive phase III. With a protocol established on ID27 for such high-pressure procedures on hydrogen, the stage is set for future developments – perhaps even past 320 GPa, beyond which no measurements, spectroscopic, diffractive or otherwise – yet exist.

ESRF celebrates two decades of science

For the 20th anniversary of the creation of the ESRF, the facility hosted a celebration day at the end of 2008. Personalities from science labs and the synchrotron world, as well as retired and current staff, gathered to evoke fond memories of the origins of the ESRF and how the facility has grown in the last two decades.

The ESRF's Convention was signed on 16 December 1988 and the facility welcomed the first users at the end of 1992, although user operation started officially in 1994. Today it has 6200 user visits a year, and in 2007 a total of 1511 papers on work at the ESRF appeared in peer-reviewed journals.

D MOREL

Akira Kira shakes hands with Bill Stirling during the ESRF's 20th anniversary celebrations. Kira is director-general of the Japanese synchrotron SPring-8, which is the largest such facility in the world.

Cryogenic magnet undulators allow greater brilliance

Magnets are the sheepdogs of particle accelerators – they herd a speeding electron towards where it is needed. Synchrotrons in particular use rows of magnets in undulators to produce highly collimated, intense X-ray beams. Currently the best-performing undulators are the so-called in-vacuum undulators. However, for this type of device, magnet materials with a high resistance to demagnetization (coercivity) must be selected. This can be achieved using neodymium iron boron (NdFeB) alloys at the expense of reduced field performances (remanence).

However, improvements could be made on both coercivity and remanence at the same time by cooling the best-available NdFeB magnets to 150 K. ESRF engineers set out to see if magnets that were enhanced in this way could be incorporated into an undulator. They were successful. The prototype cryogenically cooled permanent magnet undulator (CPMU), the first of its kind worldwide, allows four times as much brilliance at high energies (>80 keV) than current undulators.

It has been used successfully for a year, producing consistent high-quality results, and it can now be rolled out to other locations. The additional energy boost given to the photon by this type of machine will be particularly useful for other, smaller synchrotrons running at lower energies to improve photon intensities above 10 keV. The light sources Soleil and Diamond are already planning to build their own versions of the ESRF design.

For the ESRF, the beam engineers plan to produce a CPMU that is capable of an even more brilliant beam this year. Joel Chavanne, an ESRF undulator engineer, explains: "The first machine was a proof of concept; the second will be optimised to produce the best results possible." The super-high energy beams that are produced by this super-CPMU will add another unique feature to the ESRF's repertoire of world-class instruments.

Flu-virus secrets are exposed

New drugs and vaccines against influenza are desperately being sought – seasonal epidemics kill several hundred thousand people every year and a global pandemic looms if bird flu strains develop the ability to infect humans easily.

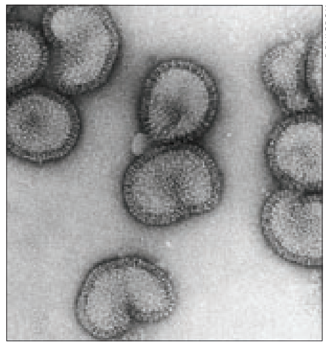
Researchers at the European Molecular Biology Laboratory (EMBL) and the Unit of Virus Host-Cell Interaction (UVHCI), jointly set up by University Joseph Fourier, EMBL and the National Centre for Scientific Research in Grenoble, France, have discovered how the influenza virus hijacks the cell's RNA molecules in the body.

The team produced crystals of crucial viral domains and examined their structure with the X-ray beams of the ESRF. The 3D structural images show on the atomic scale the location of a "knife" that is crucial to the virus's function. These findings are the culmination of a research effort that began more than 20 years ago. The breakthrough dates back to 2006 when the group succeeded in producing crystals of a suitable quality for the X-ray analysis of atomic structures.

When an influenza virus infects a host cell it steers the cell's machinery towards synthesising viral proteins rather than producing the proteins that the cell needs. To this end the virus uses the enzyme polymerase to steal a small piece of host cell genetic material (mRNA) and adds it to its own genetic code. This piece – the cap – has the function of a key, turning on the host cell's protein-synthesis machinery to work for the virus. However, which of the three suspected protein domains in the polymerase does what in the piracy remains controversial. The Grenoble team has now discovered that a protein domain called PA is responsible for cleaving the cap from the mRNA.

"Our results came as a big surprise because everybody thought that the cleaving activity resided in a different part," explains Rob Ruigrok, vice-director of the UVHCI.

"These new insights make PA a promising antiviral drug target. Inhibiting the cleaving of the cap is an efficient way to stop infection because the virus can no longer multiply. Now we know where to focus drug-design efforts," adds Stephen Cusack, head of EMBL Grenoble and director of the UVHCI.


R RUIGROK

A recent electron microscopy image of the influenza virus.

The high-resolution images of the viral domain reveal the individual amino acids that constitute the active site responsible for cleaving the RNA: the hollow canyon in the centre captures the long mRNA strand and the metal complexes at the top edges of the canyon cut off the cap. An experiment carried out at the ESRF confirmed that these contain manganese, providing an important hint for drug development.

"A key aspect of the discovery was the close distance between the institutes. The ESRF is a neighbour to the UVHCI and the Grenoble outstation of EMBL. The rapid access to X-ray beam time and the development, jointly with EMBL, of beamline automation allowed the scientists to perfect their crystals to reach the necessary quality very efficiently," says Sine Larsen, director of research at the ESRF.

Only a few months ago the same group of scientists identified the structure of another key part of the influenza–host cell interaction – a nearby domain called PB2 that recognises and binds to the cap of the host cell. Taken together, these two findings provide an almost complete picture of the cap-snatching mechanism that allows the influenza virus to take control of human cells.

Reference

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Users' corner

Users' Meeting

The 19th ESRF Users' Meeting and Associated Workshops took place on 2–5 February. During the plenary session on 4 February the keynote lecture on new results and future directions for science at high pressure using synchrotron studies was given by Paul Loubeyre from the CEA, while Dennis Mills presented a renewal plan for the Advanced Photon Source.

Following the activity report from the ESRF directors, a presentation was made by the winner of the Young Scientist Award. This year the prize went to Gergely Katona from the University of Gothenburg in Sweden for his innovative experiments in the field of structural dynamics of proteins using synchrotron radiation.

This year, two associated workshops and a school were held in conjunction with the Users' Meeting. These were:
- Energy dispersive X-ray absorption spectroscopy: scientific opportunities and technical challenges
- Structures and dynamics of soft surfaces and interfaces
- Macromolecular crystallography school: "Getting the most from the ESRF MX beamlines"


C ARGOUD

Gergely Katona (right) receives his Young Scientist Award from Gerlind Sulzenbacher, head of the Users' Organisation.


C ARGOUD

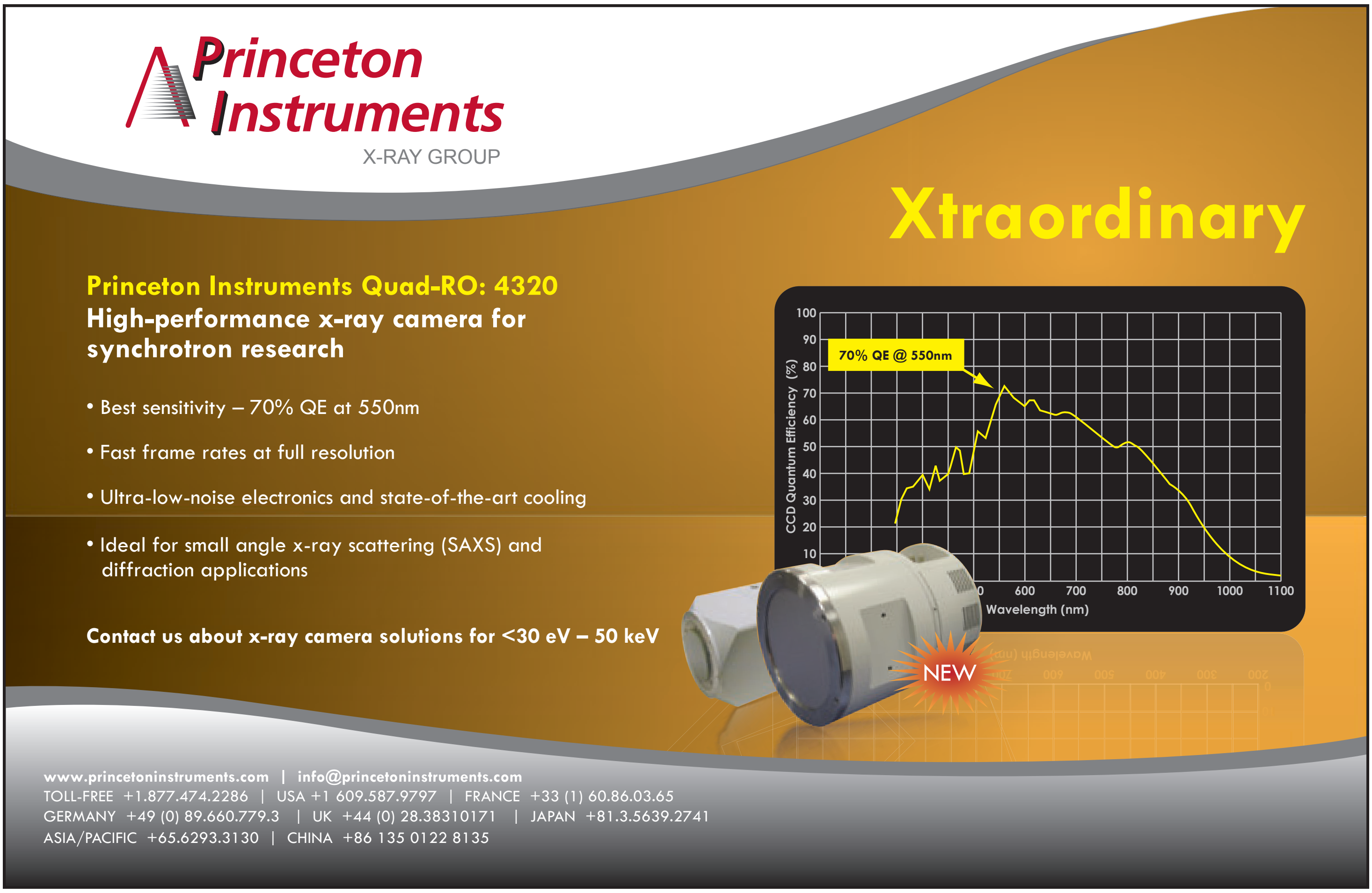
Participants from the ESRF's crystallography school, which took place within the framework of the Users' Meeting.

These events were popular and fruitful for the scientific communities concerned.

Beam time allocation

The next Beam Time Allocation Panel meeting to review proposals submitted for long-term projects and standard beamtime proposals will take place on 23 and 24 April.

- **The X-ray screening of protein crystallisation** plates and microchips is now routinely used on beamline FIP-BM30A. Beam time is available for all users who would like to test this new technique. An optimised crystallisation plate specifically designed for such use is also available. Interested scientists should contact Jean-Luc Ferrer (email jean-luc.ferrer@ibs.fr).
- **ID29 has upgraded its sample environment.** The beamline has been equipped with a microdiffractometer that will allow routine multi- and single-wavelength anomalous dispersion (SAD, MAD) experiments with microbeams down to the sizes of 50 and 15 μm, respectively. In the near future, a 5 μm beam size will also be available. The introduction of beam-cleaning apertures decreases scattering and will reduce background noise on the diffraction image.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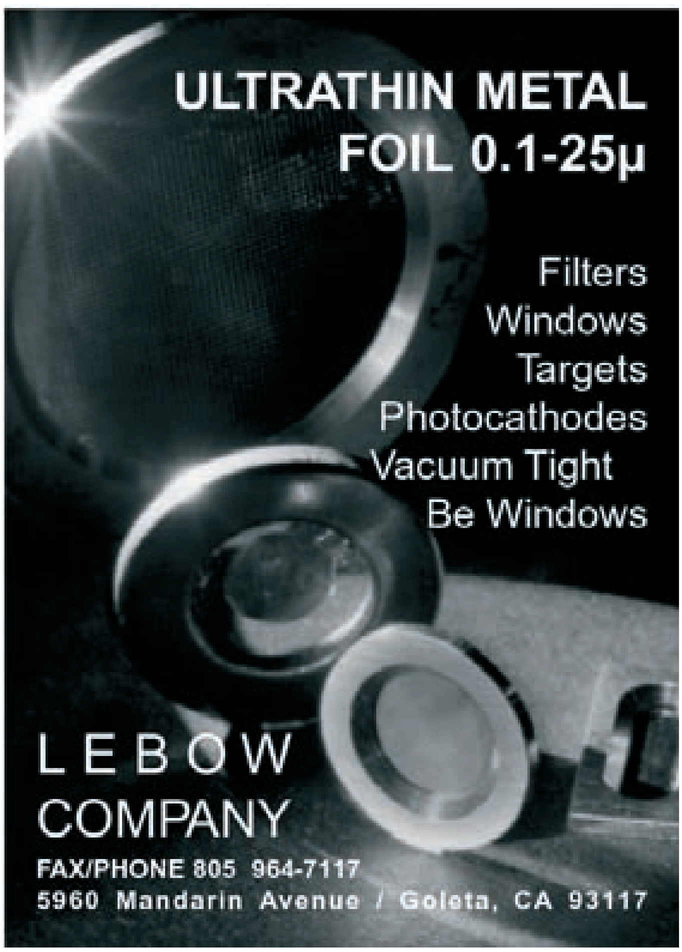
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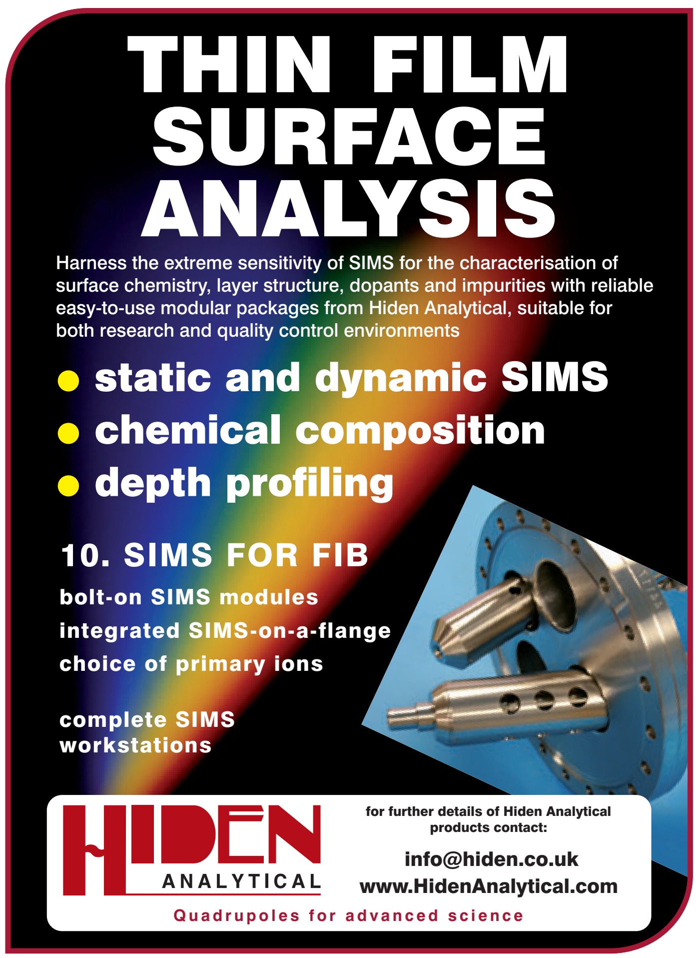
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Synchrotrons help to make water clearer

Water, despite being a ubiquitous "ingredient" in our lives and having a relatively simple molecular structure, has been the subject of controversies for years and still keeps scientists all over the world scratching their heads. Synchrotron sources are optimal tools to study it.

ISTOCKPHOTO.COM/S JASTRZEBSKI

Ingredients of life. The water molecule is a remarkable substance with exceptional features.

Despite having a simple formula, water is more complicated than it seems. It has a very low molecular weight, so it should boil at around –90 °C and exist as a gas rather than a liquid. It should also expand on melting from ice and contract on crystallising. However, this is not the case. Other exceptional features of water include its good solvent property, its strong surface tension (its tendency to resist being pulled apart) and its hydrophilic effect – in which water molecules are bound together by an attraction called hydrogen bonding. How water "sticks" together has been, and still is, the major focus of study for many scientists.

Hydrogen bonds result from the force of attraction between two atoms with different electrical charges. In a water molecule, hydrogen atoms are positively charged and oxygen is negatively charged, so the atoms attract each other, binding the oxygen from one molecule to the hydrogen of another.

Several scientists have questioned whether this hypothesis alone accounts for the attraction between the atoms in water because, they argue, these bonds are very weak. In 1935, Nobel Laureate Linus Pauling referred to the hydrogen bonds in water as covalent, meaning that there is electron sharing between molecules, making them stay together more strongly. Today the scientific community generally accepts the idea of electron sharing, but the degree to which this is responsible is in question.

Synchrotron sources have become excellent tools for researchers trying to explain the structure of water. Initially scientists used techniques such as X-ray diffraction, but

"How water 'sticks' together… still is the major focus of study for many scientists"

today's more prominent methods are X-ray absorption and Raman spectroscopy with water under confinement or extreme pressure and temperature conditions. Despite the new methodology there are still different views in the community about the structure of water.

In the traditional view, when water exists as ice, the hydrogen bonds form a complete network, with each molecule donating two bonds and accepting two bonds from its neighbours, forming a tetrahedral structure. When the ice melts it loses about 10% of those hydrogen bonds but it keeps its tetrahedral shape. In 2004, researchers from Stanford University used X-ray absorption spectroscopy (XAS) and X-ray Raman scattering to study water. They found that 80% of its hydrogen bonds were broken and stated that the molecules formed a network of chains or rings (Wernet *et al.* 2004). In XAS the absorption spectrum is sensitive to the local structure. A different interpretation of the XAS spectrum in line with the traditional tetrahedral picture of water has, however, also been proposed (Smith *et al.* 2004).

In a recent experiment a team from the University of Saskatchewan, the Steacie Institute for Molecular Sciences in Canada and the ESRF compared the X-ray Raman spectra for water, crystalline ice and two kinds of amorphous ice. They found that a clear direct connection between the spectra and the local structure is a difficult task to establish. The results made the scientists conclude: "A quantitative description of the XAS of water and ices is beyond the currently employed theoretical methods." (Tse *et al.* 2008). They alleged that the reason for this resides mainly in the incomplete description of the continuum electronic states.

MC

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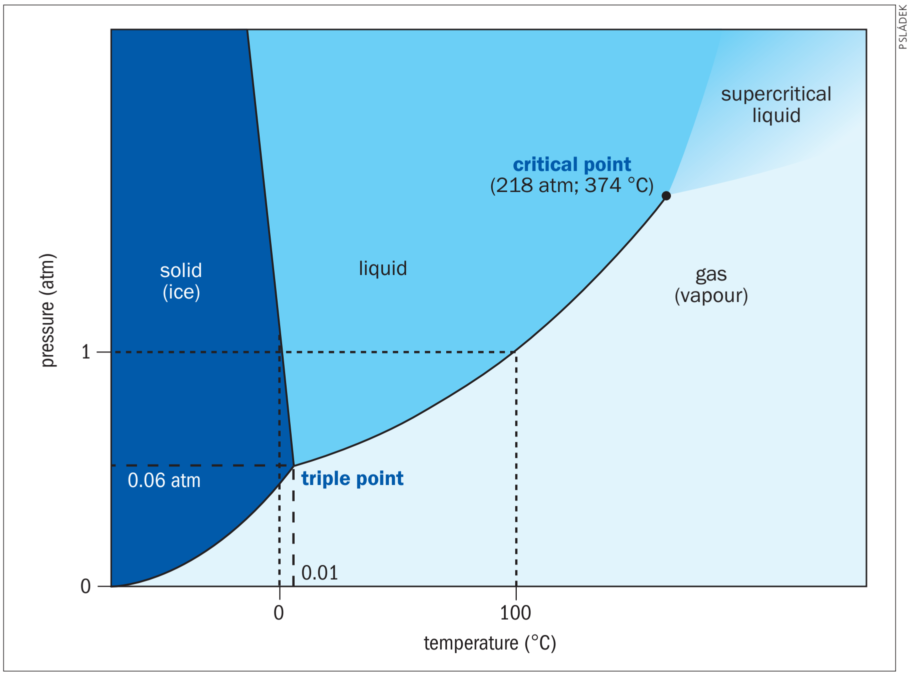
P H Wernet *et al.* 2004 *Science* **304** 995.

The future looks dynamic for H_2O

Water exists in different phases depending on temperature and pressure, and scientists are keen to gain an insight into the dynamics of H_2O as it changes phase. Researchers at the ESRF have now gained an insight into the dynamics of supercritical water.



Simplified phase diagram for water, showing the different states at various pressures and temperatures. Beyond the critical point, liquid water and water vapour behave in exactly the same manner. This is the region of supercritical fluid behaviour. In the interests of clarity, the various different forms of ice that are possible within the complex solid region are not shown.

Every secondary-school pupil studies the different forms of water, which can be represented by a phase diagram. Scientists who are working on water know the diagram by heart and use it when studying the way in which water changes as they increase pressure and temperature.

In the phase diagram there are points where phase-consistence lines join, when three phases coexist but may abruptly change into each other if there is a slight change in temperature or pressure. Critical points occur at the end of a phase-consistence line, where the properties of the two phases become indistinguishable from each other – for instance, when liquid water is hot enough and gaseous water is under sufficient pressure that their densities can be identical.

Different approaches

To investigate the dynamics of water, theoreticians use molecular dynamics simulations whereas experimentalists apply high-frequency spectroscopies, such as neutron or X-ray scattering.

Previously, scientists have shown that the microscopic mechanism responsible for the main relaxation process is the continuous rearranging of the water in the hydrogen-bond network. However, scientists at the ELETTRA synchrotron in Trieste, CRS SOFT-INFM-CNR in Italy and the ESRF have recently managed to monitor the changes in water while they altered the temperature from ambient to supercritical conditions. The team characterised the dependency on momentum, temperature and density of the active relaxation processes of water.

In particular, the researchers who used the ESRF's inelastic scattering beamline ID28 found that the relaxation mechanisms in water change as it goes from liquid to supercritical conditions. This is related to viscoelastic effects on the acoustic dispersion, which gradually disappear when going from liquid to supercritical water. This effect reveals that, in the liquid phase, the relaxation is dominated by the making and breaking of intermolecular bonds, whereas in the supercritical region it is governed by binary intermolecular collisions.
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When ice vibrates

Amorphous ice, in its different forms, also exhibits complex vibrational dynamics. Inelastic X-ray scattering has recently been used to study this. A team from the Institut Laue Langevin, the universities of Darmstadt and Dortmund, and the ESRF has investigated the dynamics of very-high-density amorphous ice samples. Previous studies provided an insight into samples of low-density and high-density amorphous ice, but not very-high-density amorphous ice. The scientists observed crystal-like phonons – excitations of longitudinal and transverse polarization, as well as of acoustic and optical character. An averaged longitudinal velocity of sound of about 4050 m/s was established, exceeding the values obtained for the lower-density amorphous ice modifications reported previously. In general, the results obtained from this study indicate a more pronounced homogeneity of the matrix of very-high-density amorphous ice compared with that of high-density amorphous ice.
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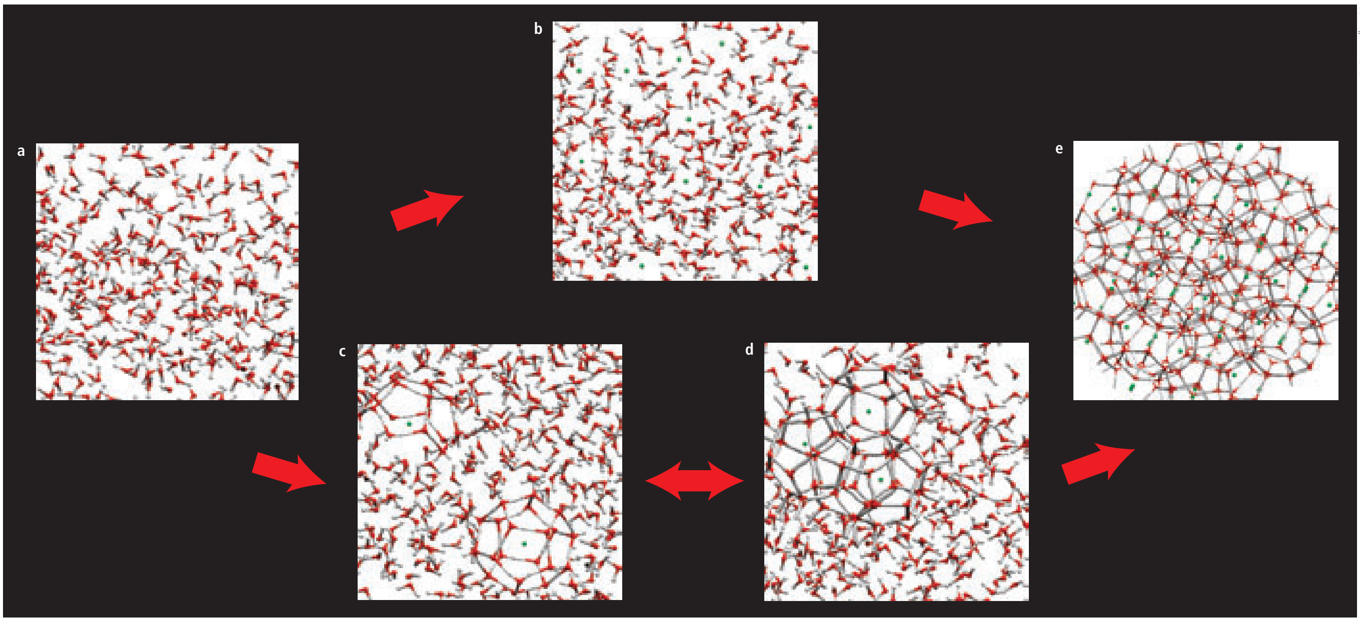


Two theories to explain the formation of hydrates. Comparison of the cluster nucleation theory (a, c, d, e) and the local structuring hypothesis (a, b, e). a) The structure of water without dissolved gas molecules (initial condition). c) A cluster forms immediately after the dissolution of gas molecules, and d) later the cluster pre-stages agglomerate by sharing faces. These agglomerated clusters may be unstable, so they may go back to a step before. In the upper example (a, b, e) there is no cluster formation after the dissolution of gas molecules. e) Hydrate nucleation.

Scientists look inside ice-like water that stores gas

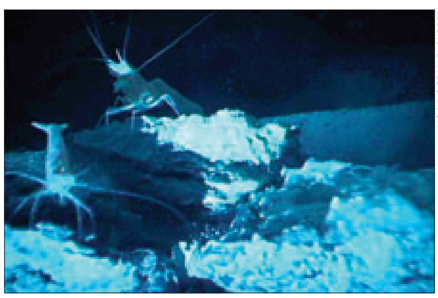
Scientists in Germany and France have determined the structural formation of hydrates (solid water), which may prove useful for the environmentally friendly storage of CO_2 or H_2.

Water could contribute to gas storage in a solid phase, which is called clathrate hydrate. This form of water typically appears at low temperature and high pressure. It resembles ice and contains gas molecules trapped inside cages of hydrogen-bonded water molecules. The ocean floor and permafrost areas offer the perfect conditions for hydrates to form. Those on the seabed store large quantities of methane, and scientists are considering these solids as an environmentally friendly solution for carbon dioxide (CO_2) or hydrogen storage.

It's still not clear how hydrates form at the microscopic level. There are currently two models. The first states that gas is dissolved in water and forms some pre-cages (clusters). When these reach a critical size they form the hydrate. The second model holds that there is no special arrangement around the dissolved gas molecule in the hydrate's formation steps.

Scientists from the Technische Universität Dortmund, HASYLAB in Germany and the ESRF have analysed the structure of the CO_2–water interface in conditions where a gas hydrate can be formed. They studied the interface with both gaseous and liquid CO_2.

First the researchers looked for hydrate formation at the water–gaseous CO_2 interface. They used X-ray reflectivity at the ESRF to investigate the formation of thin layers on the water. According to the cluster-nucleation theory, the formation of clusters would make the surface rough. However, the scientists could only find a thin layer of CO_2 at the water's surface, which did not trigger the gas hydrate-formation process.



A couple of shrimp crawl over an outcrop of gas hydrates on Blake Ridge off the east coast of the US. The animals may be grazing on bacteria living on the surface of hydrates.

Next they decided to apply more pressure to the samples – up to a level above the condensation pressure of CO_2. This made the CO_2 change to a liquid. This time the scientists used X-ray diffraction at ESRF and at DELTA in Dortmund. They found Bragg reflections of CO_2 hydrate. After waiting several minutes they performed more scans, which showed a dynamic behaviour among the formed clusters. More than 90 minutes later the dynamics were still visible.

"We think that the formation and non-formation of the CO_2 hydrate at the different interfaces suggest a random formation mechanism without hydrate precursor," explains the team's leader Felix Lehmkühler from the TU Dortmund. "We used the ESRF beamline ID15 because of the unique set-up for liquid surfaces. It is the only place in Europe that allows these kinds of experiment."

Lehmkühler adds: "This new knowledge can be useful for technological applications such as CO_2 and hydrogen storage in hydrates, and the inhibition of hydrate formation in pipelines." The team's next challenge is to study other hydrates and also the evolution of the hydrate-formation process.
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Reference

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Ice crystals feel the pressure

A team of Grenoble-based scientists is trying to determine exactly how ice crystals deform when subjected to an applied stress. Understanding the deformation structures of ice is important not only in terms of environmental modelling but also for materials science.

The polar ice caps and glaciers are crucial elements of the Earth climatic system because they have a direct and major influence on the circulation of global atmospheric winds and oceanic currents. Therefore modelling how these ice masses move and deform in response to climate changes is essential.

The mechanical properties of crystals are controlled by the presence, movement and creation of linear crystalline defects called dislocations, which allow ice crystals to deform under applied stresses. The way in which dislocations move in ice crystals is directional, being very easy within the "basal" plane of the hexagonal structure (figure 1a) and rather difficult in directions perpendicular to this plane. Under shear stress, deformation mainly occurs by gliding along "slip" basal planes, where dislocations move or are created (figure 1a). Dislocation motion and multiplication can be studied *in situ*, under an applied stress, using X-ray diffraction topography at synchrotron sources. The investigation of single crystals is a mandatory first step when studying ice.

However, ice occurs in most situations as a polycrystal, where grain boundaries act both as effective sources of lattice dislocations and as strong obstacles to dislocation motion. When a polycrystal deforms, strain incompatibilities arise at grain boundaries owing to the single crystalline grain's directional deformation: each grain cannot deform in isolation because its neighbouring grains constitute an additional constraint (figure 1b). These incompatibilities at grain boundaries generate stress concentrations that provoke intragranular strain heterogeneity. Studying strain incompatibility at a grain boundary and intragranular strain heterogeneity are important in explaining strain-hardening and fracture processes.

The simplest model for a polycrystal is a tricrystal (figure 2), which exhibits grains with different crystalline orientation and grain boundaries meeting on a triple point, while at the same time remaining simple enough to allow the elaboration of a model from the experimental results. A team from the Laboratoire de Glaciologie et Géophysique de l'Environnement de Grenoble, led by Armelle Philip and Jacques Meyssonnier, has succeeded in growing high-quality tricrystals of ice. Figure 3 shows Bragg diffraction images of one of these tricrystals during the early stages of compression, recorded by the team at ID19 in collaboration with ESRF staff.

To carry out the experiments, the team designed and commissioned a special device that allowed them simultaneously to keep the sample at low temperature, apply an increasingly large uniaxial stress in a controlled way, illuminate the sample with X-rays and

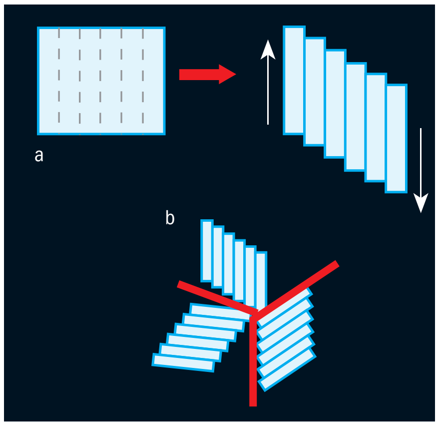

Figure 1: a) directional deformation of a crystal of ice, and b) strain incompatibilities occurring when several grains are deformed in a polycrystal.

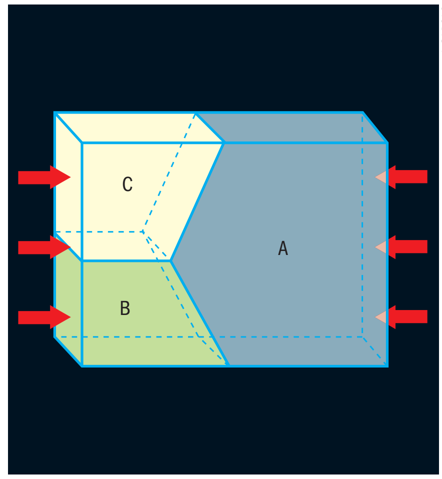

Figure 2: a tricrystal, the simplest model for a polycrystal, when under compression.

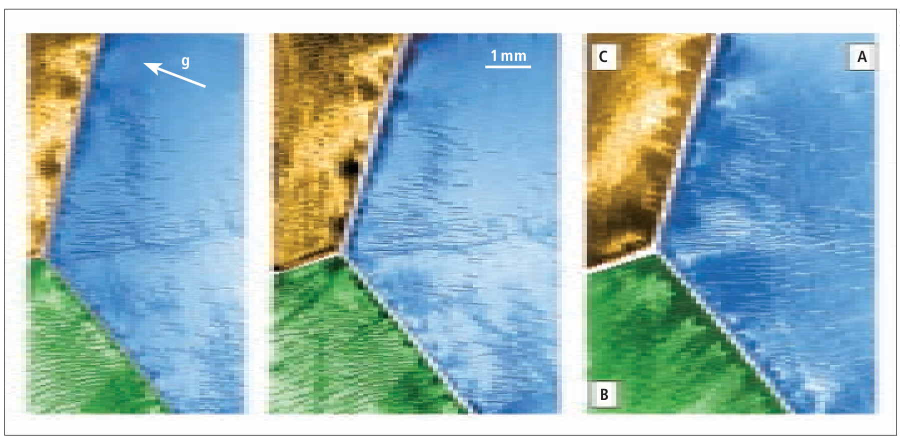

Figure 3: Bragg-diffraction composite image (the reflection used is different for the three grains) of various steps of the deformation of an ice tricrystal under compression (the direction is nearly parallel to the boundary between grains B and C). Before compression (left), under 0.24 MPa (centre) and under less than 0.36 MPa (right).

M CAPELLAS-ESPUNY

When a polycrystal deforms, each grain cannot deform in isolation because its neighbouring grains constitute an additional constraint.

record the diffracted images on a 2D detector. Colour was added to the images (figure 3), with each associated with one of the grains (A, B and C) in figure 2. The diffraction vector, g, is indicated for the main grain (A). The result is a series of dislocations, which show up as lines, are already present in the nondeformed state and move (compare A and B) when stress is applied. Many new dislocations develop when the sample is further deformed (grain A). Grain boundary regions deform before the interior of the grain. These regions (darker areas in the image) concentrate heterogeneously on the boundaries and are transmitted to the neighbouring grain when a greater load is applied.

The final goal of this *in situ* synchrotron radiation Bragg-diffraction imaging work is to build X-ray-imaging techniques for a predictive theory of the deformation of a small volume of polycrystalline material, in particular ice. This is achieved through the study of the crystal microstructure's evolution during loading carried out by a large scientific collaboration that includes specialists in ice as well as mechanics.

To obtain significant results, the team is developing a fully quantitative procedure on BM5. On this beamline the scientists will combine X-ray imaging for the location of the deformed regions and X-ray diffraction, which enables local measurement of the distortion (and hence the density of dislocations), with a spatial resolution in the few tens of microns range. The observations will be compared with the results of models that simulate the dislocation movement, taking into account its interaction with the stress fields generated by the surrounding dislocations and by the boundary conditions. Once complete, this work will represent a step towards improving the modelling of polar ice sheets that exhibit a continuous evolution of the ice microstructure with depth.

In parallel to this fundamental work a study of the deformation mechanisms of snow is ongoing. The aim is to assess the influence of the microstructure of snow on its mechanical behaviour by observing how it deforms at the grain scale in the regime where fractures are not present. In particular, the focus is on the relative influences of intragranular-viscoplastic deformation versus grain-boundary sliding.

For this purpose *in situ* compression tests on snow are monitored by two complementary synchrotron radiation X-ray imaging techniques: X-ray microtomography in absorption mode, and a new technique called diffraction contrast microtomography (DCT), developed at the ESRF. By analysing the diffraction spots from the ice crystals that happen to be under Bragg conditions during the rotation of the snow sample, it is possible to determine simultaneously the 3D shapes and crystallographic orientations of the grains. This is essential in view of realistic numerical simulations of the snow-deformation experiments (i.e. simulations that account for the anisotropy of ice). The first experimental results have been obtained from snow samples made of refrozen wet grains, presenting a limited number of grains and producing large diffraction spots that are convenient for the validation of DCT. Besides the crystallographic orientations of the crystals, other useful information given by the technique concerns the lattice distortion of the crystals, which indicates the degree of intragranular deformation experienced by the snow sample on a grain-by-grain basis.

"The investigation of single crystals is a mandatory first step when studying ice"

● This is collaborative work, led by Jacques Meyssonnier (LGGE) within the framework of the French ANR "Snow White" project. It is a joint effort with the Centre d'Etudes de la Neige, the Laboratoire 3Sr and the Cemagref – all in Grenoble – with a strong involvement by the ESRF X-ray Imaging Group.
J Baruchel

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SUD ARCHITECTES

A future bird's-eye view of the facility. This is an artist's impression of what the ESRF may look like once the Upgrade Programme is complete.

Plans to upgrade beamlines are starting to take shape

Since the latter part of 2008, ESRF management and staff have been working with the user community to determine the details of the Upgrade Programme. The users are playing an important role in producing a scientific case for the upgrade of beamlines.

Seven years is the lifetime of phase I of the Upgrade Programme, which the Council approved at the end of 2008. This means an increase by 10% of the ESRF budget every year, with a total of €177m. These funds will allow a refurbishment of all beamlines, and eight new ones will be constructed, together with the technology that they need (e.g. optics, accelerator and X-ray source complex). The creation of these new stations is being addressed by ESRF scientists and external experts (many of whom are regular users).

Brainstorming sessions, funded by the European Commission FP7 grant, are used to build the science cases and explore the technological limits of the 11 candidate beamlines, which helps to define the necessary detailed, technical design reports. Further guidance on the science of the new beamlines will be provided by the Scientific Advisory Committee at its meeting in May.

C ARGOUD

Planning a beamline. The committee discusses UPBL7, a facility that would be unique among synchrotrons. Typically, brainstorming sessions involve a couple of days of intense discussion.

Beamlines of the future

As part of phase I of the Upgrade Programme, 11 beamline proposals are under discussion:

UPBL1 local probe coherent diffraction imaging and nanobeam diffraction for the characterisation of individual nanostructures

UPBL2 high-energy beamline for buried interface structure and materials processing

UPBL3 nuclear resonance beamline for the study of nanoscale materials: the interplay of growth, structure, electric and magnetic properties, as well as dynamics

UPBL4 beamline for imaging, fluorescence and spectroscopy at the nanoscale

UPBL5 beamline for parallel and coherent beam imaging

UPBL6 high-energy resolution inelastic scattering in the hard-X-ray range with micro- and nanofocus capabilities

UPBL7 soft X-rays for nanomagnetic and electronic spectroscopy

UPBL8 nano- and microbeam crystallography for structural and functional biology and soft matter

UPBL9 (a) submicroradian angular resolution small-angle scattering for probing the structure and non-equilibrium dynamics of self-assembling soft matter and biological systems; (b) structural dynamics of molecular assemblies

UPBL10 large-scale automated screening, selection and data collection for macromolecular crystallography

UPBL11 pushing the limits of X-ray absorption spectroscopy for time-resolved applications and studies at extreme conditions.

The first discussion was dedicated to a beamline for time-resolved and extreme-condition X-ray absorption spectroscopy, UPBL11, which could push the boundaries of research in Earth and planetary sciences, catalysis and materials science.

One of the areas where it is expected to have a significant impact is catalysis. Some 90% of all commercially produced chemicals involve catalysts at some stage in their production, according to *R&D* magazine. Car manufacturers are investigating how to improve these agents in the hope of being able to develop less-polluting cars, and UPBL11 may provide the answer.

At the ESRF, scientists have already studied catalysts under real working conditions, but UPBL11 would allow them to do it more effectively. The current systems, such as three-way catalysts, are made of four or five chemical species. UPBL11 would allow researchers to study the fast changes occurring around each of the species during a reaction in dilute samples (those of interest to the car industry), and to obtain more accurate information on a wider range of elements, as well as at much shorter timescales.

This should make it possible to get more accurate information about the relationship between the activity of the catalyst and its structure. This should in turn help to find the right elements and composition to generate materials with the desired properties.

Another example of the promise of the new beamline is in the study of melted metals at extreme pressures and temperatures, simulating the thermodynamic conditions at the Earth's core. New insight into the melting of iron (the most abundant metal in the Earth) and its alloys will provide valuable information about the chemistry inside our planet. UPBL11 will be designed to follow chemical reactions in these extreme conditions, which will provide key information about the processes that occurred during the formation of planets.

During the initial brainstorming, experts recommended to push the time resolution to the microsecond level for non-reversible processes. They proposed the rapid adoption of a double-branch scheme so as to increase the availability of the beamline, which is limited due to the complexity of set-ups of the experiments. They also requested software development for handling large data volumes.

The Macromolecular Crystallography Group's bid for the Upgrade Programme is UPBL10 – a next-generation, highly automated, high-throughput facility to evaluate the many thousands of crystals that each of their projects produce. This would cater for scientists undertaking ambitious work, such as the study of complex membrane proteins and large macromolecular assemblies.

An example of the former is G-protein coupled receptors, which constitute the largest family of this kind of protein in the human genome and are involved in controlling physiological processes. External experts clearly stated at the initial meeting that the ESRF is the optimal place to develop this kind of project because its beamlines have already achieved a lot of automation and, also, because of the size and scope of the facility.

UPBL10 would comprise four high-intensity X-ray beams: three to evaluate the different types of crystal and one specialised beam to collect the diffraction patterns from these very small or disordered crystals. Samples sent to the ESRF would be sorted and mounted automatically by robots. Complex software would then determine from the images of the crystals which were the "best" samples.

The facility is expected to increase fivefold its capabilities to evaluate samples (today it processes 120 000 samples a year). The ability to identify the "needle in the haystack" – those "one in a thousand" samples that are well ordered – will enable new science and new projects to be performed.

State-of-the-art soft-X-ray beamline

UPBL7 is the name of a proposed resonant inelastic X-ray scattering beamline with very-high-energy resolution and high-quality X-ray magnetic circular dichroism. The brainstorming meeting for this beamline not only gathered users, external experts in the relevant fields and ESRF staff, but also experts in theory or complementary experimental fields, such as neutron scattering.

This new beamline would replace the current soft X-ray beamline, ID08. Its deployment would focus on magnetism and electronic properties of matter, and it would tackle some of the questions that remain unanswered. A key research area would be the study of the magnetism and electronic structure of strongly correlated materials, and, in particular, spin, orbital and charge degrees of freedom in these materials.

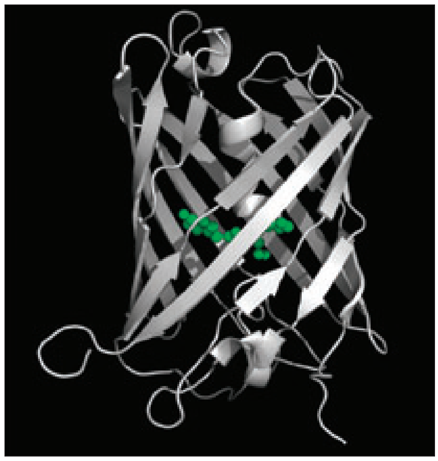
UPBL7 would be different from the beamlines currently in synchrotrons, mainly due to the unprecedented energy resolution that it is expected to have, as well as the range of new possibilities that it will offer for the sample environments. The option of being able to exploit a high-magnetic-field facility (>30 T) was positively received at the meeting.

A chance discovery: a new unique fluorescent protein

An attempt to study fluorescent proteins (FPs) reveals a third form of photoactivatable FPs.

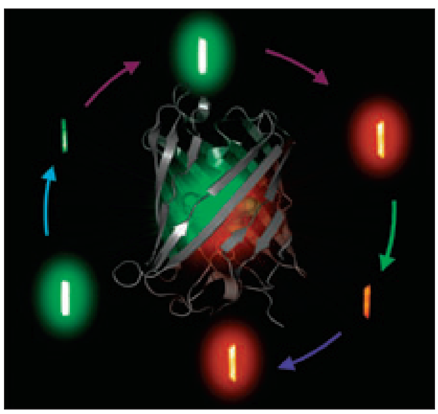
It did not look like the best of days at the lab. Virgile Adam had problems crystallising samples from corals sent to him by a team from Ulm in Germany. His intention was to study green fluorescent proteins, which are used to visualise molecules inside cells. Frustrated, he asked Guillaume Desfonds, a trainee at the ESRF, to irradiate another mutant of the sample that had been sent to him, and that they had just crystallised, directly under sunlight to see how the photosensitive protein would react. It exhibited odd behaviour, undergoing different phototransformations depending on the lighting conditions.

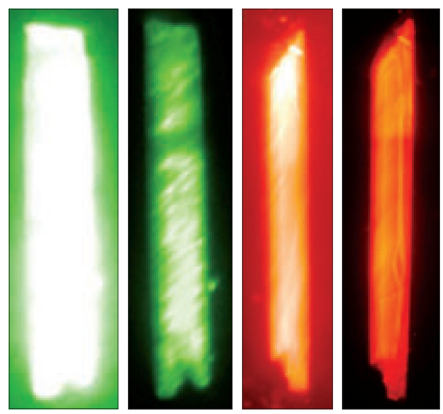
Adam decided to irradiate crystals of the protein with different lasers to determine which wavelengths were crucial. When using cyan light, he noticed that the crystals quickly and completely lost their colour. He wanted to take a snapshot of them, but there was no camera available. On the following day he arrived at the lab, ready to take a photo, and, to his surprise, he saw that "the crystals had come back to life".



The cryobench

The cryobench laboratory was used by the IrisFP team to perform UV-visible spectroscopy on the protein crystals. It comprises a microspectrophotometer – a piece of apparatus that allows the user to take absorption, fluorescence and/or Raman measurements directly from a protein crystal. The cryobench allowed the scientists to correlate structure, function and mechanism in IrisFP. It combines crystallography and optical spectroscopy, and it is now available to users either offline (as a standalone machine) or online (on the MX beamlines).





V ADAMS

IrisFP undergoes multiple colour changes, which makes it a powerful tool for bioimaging and biotechnological applications. Top left: the protein's X-ray structure (grey ribbons). Bottom left: the green and red rays represent multicolour light emission, while pictures of crystals of IrisFP in its different colour states are shown round the central image (and bottom right), linked by arrows representing the colours of the lasers needed to induce the colour changes.

A new family member

Fluorescent proteins (FP) are widely used in cell imaging as biological markers. They are like highlighters that scientists attach to a molecule that they want to follow in the cell. Many research teams around the world try to design and optimise hundreds of FPs with different colours. Some of these markers, such as the original green fluorescent protein (GFP), are found in nature (e.g. jellyfish and corals), but many others have been genetically engineered. Recently, researchers discovered photoactivatable FPs (PAFPs). The colour of these can be changed at will by using the appropriate lasers. They have triggered something of a revolution in the field of optical microscopy, raising the possibility of breaking the diffraction barrier – in other words, imaging biological samples with an accuracy of about 10 nm using visible light.

Until Adam went to the lab the day after irradiating his mutant samples, there were two distinct families of PAFPs. There were those that, when irradiated with visible light, switch to a dark state, and then switch back to a bright state when irradiated with ultraviolet light. This effect is reversible, so the protein can be switched "on" and "off" at will. There were also green PAFPs that, when excited with ultraviolet light, turn red irreversibly. To advance super-resolution imaging, scientists search for PAFPs with the best properties.

The protein that Adam and his team were studying exhibited a behaviour that is different from the two known families. It can be switched reversibly between fluorescent and non-fluorescent forms in its green state, then photoconverted from green to red, and finally switched reversibly between fluorescent and non-fluorescent forms in its red state. It has been named IrisFP. "Iris is the Greek goddess who personifies the rainbow, which refers to the multicolour of this protein," explains Adam, who is finishing his PhD.

The team, from the Institut de Biologie Structurale (IBS), the University of Ulm and the ESRF, characterised the structure and spectroscopy of IrisFP using several macromolecular crystallography beamlines at the ESRF and the ESRF-Institut de Biologie Structurale cryobench lab.

The protein will help to overcome some drawbacks of current reversibly photoswitchable FPs, which are not visible in their off state, and of photoconvertible FPs, which are limited by the nonreversible nature of photoconversion. However, its applications won't be limited to cell biology. "We could also imagine, in the future, that IrisFP will be used in mass storage media, combining read-only and rewritable capabilities," says Dominique Bourgeois from the IBS.

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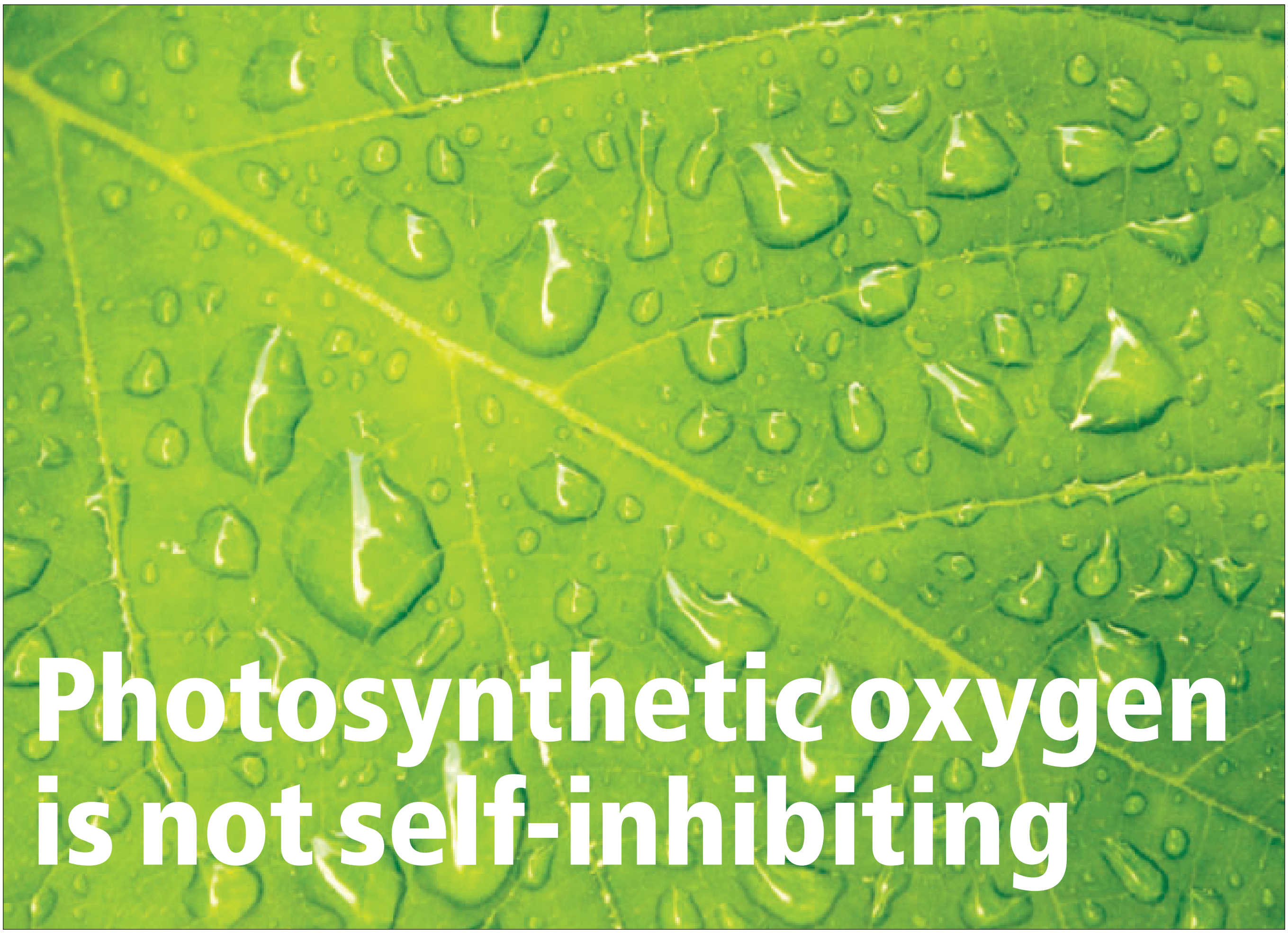

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Photosynthetic oxygen is not self-inhibiting

Inspiration from plants. By studying photosynthesis we may find new ways to tackle the problem of dwindling energy-generating resources.

Oxygen generated during photosynthesis does not inhibit the oxidation catalyst. This discovery may lead to the creation of more-effective synthetic catalysts for use in energy generation.

Photosynthesis is the ultimate solar power – that alchemy whereby plants are able to produce food and oxygen using water, carbon dioxide and sunlight. This is the chemical factory responsible for producing the atmosphere that we benefit from today, by lowering carbon-dioxide levels and raising the percentage of oxygen.

This effect runs both ways, however. Although photosynthesising plants reduce the amount of carbon dioxide in the atmosphere, this drop in carbon-dioxide levels in turn reduces the rate of photosynthesis, thereby creating a negative feedback loop. What has remained unknown, until now, is how the increased amount of oxygen produced by photosynthesis affects the efficiency of the oxygen-formation reaction.

Having extracted the protein complex photosystem II from a sample of spinach, a team from Freie Universität Berlin in Germany used beamline ID26 to watch it at work. After the protein was excited with a series of 1 ns laser flashes, X-ray absorption near-edge spectra were recorded. These allowed the group to measure the evolution of the system's oxidation states during the flashes, thereby building up a picture of what was happening over time.

Each flash "stepped" the system through one of the four well characterised stages of the Kok cycle. (Earlier work at the ESRF by the same team discovered a fifth intermediate stage.) In this cycle, two water molecules undergo oxidation to form diatomic oxygen, catalysed by a tetramanganese calcium complex bound to the photosystem II protein complex.

It had been suggested that the presence of more oxygen in the ambient environment would shift the equilibrium between the water and the oxygen to the former by a thermodynamic effect, thereby inhibiting the overall action of the catalyst. However, although an oxygen pressure of up to 16 bar does affect the redox chemistry of the reaction, the time resolution provided by the laser and X-ray experiment showed that the rate of oxygen production and the resulting yield are both unchanged by the oxygen pressure.

Limitations on plant growth in an environment with a high concentration of oxygen may come from the operation of diverse oxidative processes, but presumably not from the inhibition of the last step in the formation of oxygen. It remains to be shown whether this resistance to inhibitive effects has evolved as the atmosphere has become more oxygen rich, or whether this has always been a feature of the Kok cycle.

The next step in the investigation will be to use time-resolved X-ray-emission spectroscopy at beamline ID26 to address changes in the electronic structure of the manganese complex, aiming at a more complete mechanistic picture of the water-splitting chemistry. The results may help in the construction of more effective synthetic catalysts that can be used in the generation of future energy supplies.

K Oliver

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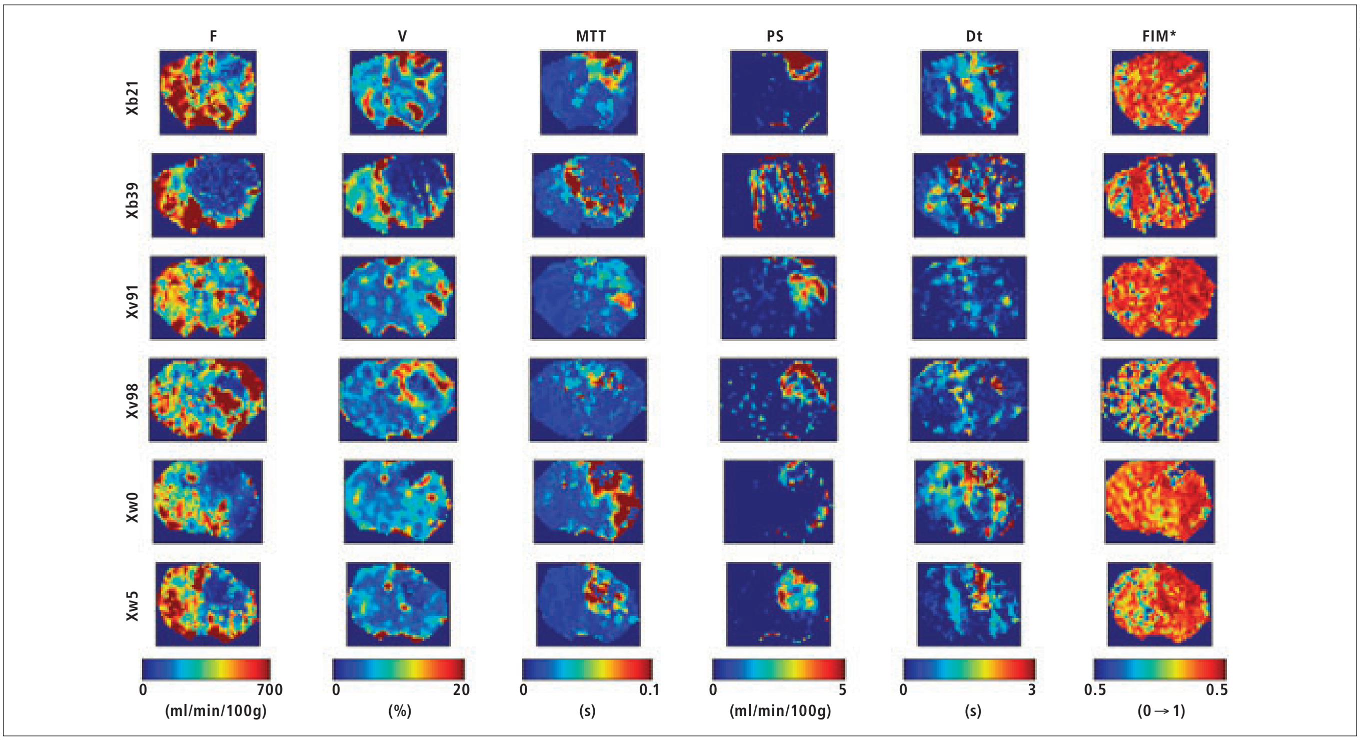

Rats with brain gliomas following the injection of contrast medium iomeprol. Following the rats' names on the far left, the five columns show physiological maps (F: blood flow; V: blood volume fraction; MTT: mean transit time; PS: permeability surface product; and Dt: time delay). Next are the reliability criteria, FMI. The colour scale for each parameter varies depending on the values: red corresponds to high values and blue to low. In the FMI maps, a red pixel has a value of 1, showing the model adjustment to be very reliable.

Software and X-rays track down tumours

There is still no gold standard for analysing the microvascularisation of a tumour *in vivo* in the same way that histology is able to achieve it *in vitro*. However, advances at the biomedical beamline are beginning to show some promising medical results.

Gliomas are aggressive brain tumours that result in an average survival time of patients of only a year, even when surgery and radiation therapy are employed. Linked to tumour growth and aggressiveness is "angiogenesis". This process involves growing new blood vessels from existing ones. In a tumour the blood–brain barrier is disrupted and this results in large areas of necrosis (where tissue begins to die and the blood is therefore unable to circulate properly).

Physicians use computed tomography (CT) and/or magnetic resonance imaging (MRI) during the injection of a contrast agent (employed to enhance the visibility of blood vessels) to map blood vessels, but both methods have limitations. The MRI signal is influenced by many parameters, and the measurements are indirect and relative. CT measurements can be directly linked to the contrast agent concentrations, but the broad energy spectrum of the X-ray tubes on hospital CT scanners can hamper the results.

A French team from the Université Paris Descartes, Hôpital Européen G Pompidou, Université Joseph Fourier, CHU de Saint-Etienne and the ESRF have developed a method to characterise the gliomas.

Synchrotron radiation CT uses a monochromatic beam and has provided the scientists with accurate and absolute measurements of the concentration of contrast agents such as iodine.

The team created a piece of software (PhysioD3D) that tests different mathematical models used in hospitals and research. The aim is to select the most relevant approach for understanding the development of cancer. "The quantification can be performed in most centres but the comparison between hospitals is limited as a result of the variety of equipment and software. PhysioD3D offers the possibility of standardizing the analysis," says Géraldine Le Duc from the ESRF.

The performance of the software depends on accurate data, which are obtained by using a monochromatic synchrotron source.

This technique is still far from being used in hospitals because of its limited accessibility. However, the team concludes (Balvay *et al.* 2009): "It is very probable that, over the next few years, compact, intense and monochromatic X-ray sources operating in the hard-X-ray regime will provide access to practical diagnostic imaging devices."
MC

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Francesco Sette: ready for adventure

The new director-general at the ESRF has a clear view of his priorities in his new position.

He enjoys reading many books simultaneously, in three different languages, and he doesn't get confused with the plots – he has great fun with it. Such an attitude corresponds to somebody who is ready to engage in many different domains with enthusiasm. The new director-general of the ESRF, Francesco Sette, who took up his position in January, is settling smoothly into his new role and he clearly knows where he would like the ESRF to go.

"It feels great to be here," he says. Just a few weeks after his arrival in the director-general's office and still with a relatively bare desk, Sette seems to enjoy his new job. He says that he considers the post an honour and a challenge. He is where he is now thanks to many circumstances – for example, previous ESRF directors who believed in him: Massimo Altarelli, who suggested that he came to the ESRF; Ruprecht Haensel, who hired him; Yves Petroff, who always supported his science, "even if he argued that my projects were too expensive"; and Bill Stirling, with whom, he says: "I spent seven wonderful years in which I tried to grow as a manager."

However, the most important reason for him is his never-ending enthusiasm to be part of an adventure at the ESRF – a place that has never stopped growing in the last 18 years, thanks to his ESRF colleagues, the ESRF users and also to the prudent but generous support of the ESRF member countries during these years. He stresses the importance of the quality of the staff in running the ESRF and his plan to have all of the employees on board in its new endeavours. His first challenge is to make the Upgrade Programme a reality while keeping the operation of the facility at its best.

Sette is no stranger to the Upgrade because he worked actively in its design as director of research. For him it constitutes a "generous, punctual reinvestment, necessary to cope with the evolution of science and to keep the ESRF attractive to the scientific community". The way to proceed with it is straightforward, he says: "I would like to efficiently combine the launch of this programme with the commitment to continue providing the best user support."

He is convinced that, to improve things, changes are a must. Among these are the construction programme and the adaptation of the internal structure of the ESRF to the Upgrade. He says that it is only possible to go forward through a collective effort. He is committed to developing a vision so that people can accept a challenging period with the prospect of a better time ahead. "One should not be afraid of changes," he concludes.

C ARGOUD

The directors' meeting. Every fortnight the directors of each of the divisions gather to discuss current matters relating to the facility under the direction of the director-general. Left to right: Manuel Rodríguez Castellano, head of the director-general's office; Pascal Elleaume, director of the accelerator and source division; Harald Reichert and Sine Larsen, directors of research; Angelika Röhr, director of administration; Rudolf Dimper, head of the computing services division; Pierre Thiry, head of technical services division; Karen Clugnet, PA to the director-general; and Francesco Sette, director-general.

The director-general in a nutshell

Francesco Sette was born in Rome, Italy, in 1957, where he obtained his PhD in physics in 1982 summa cum laude.

In 1983 he moved to the US and became first assistant scientist at the National Synchrotron Light Source at Brookhaven National Laboratory and then staff scientist at AT&T Bell Laboratories in Murray Hill. With C T Chen he opened the field of modern very high-energy resolution soft-X-ray spectroscopy with synchrotron radiation.

He joined the ESRF in 1991 to develop the very high-energy resolution inelastic X-ray scattering group and became director of research in 2001. He took up the position of ESRF director-general at the beginning of this year. He is a member of many scientific committees around the world.

The former director of research explains that the priorities in his new job are very different from those in his previous appointment and, in a way, more diversified: "I now feel responsible for the whole ESRF, which means that I am discovering and getting involved in many other aspects of the facility, such as the accelerator and its operation, the realisation of the new Experimental Hall, as well as personnel and financial issues." His job is to bring all of these aspects together and merge them into a sustainable programme, "and this is very interesting", he says.

This does not represent a move away from science. In fact, he says: "I ask myself all the time the same question: What is the scientific case and where is its added value for our user?" Sette is a member of scientific advisory committees and councils of different light sources around the world, and he intends to continue to follow technical and scientific developments in the light source community. In the future he thinks that the use of light sources will increase and that tabletop sources can help to make synchrotron radiation more available at universities, laboratories and hospitals, and therefore continue to justify centres of excellence like the ESRF for many years to come.

Two decades ago, Francesco Sette's life was driven by science, "almost to an excessive point". Today, despite long hours at work, he enjoys spending time with his wife and four children. In his free time, he visits art exhibitions, goes to the cinema and theatre and listens to music of all kinds, as well as reads books and takes part in outdoor sports. "If somebody had told me 20 years ago that I would be director-general, I would have said: 'I hope not.' I have since realised that another great challenge that gives a lot of satisfaction, apart from research, is to enable a large number of people to do science."

MC

ESRF helps scientists to build their careers

Working at the facility is a great experience for any scientist, even if their time there is limited.

Most of the researchers working at the ESRF are only around for a limited time due to the facility's strict turnover policy. This means that, as a general rule, the maximum contract a scientist can secure is only five years, and this cannot easily be extended.

The aim of this policy is to ensure that as many scientists as possible gain experience working in this unique facility, while ensuring a fresh supply of perspectives and ideas. Critics of this policy may argue that this practice can limit the scope of long-term projects and lead to a constant outflow of expertise. Whichever side of the fence you sit on, most scientists find their ESRF experience worthwhile.

Richard Davies is a scientist working on the microfocus beamline, ID13, and he will be finishing his contract in a few months. He feels that his time working at the ESRF has been very rewarding. "It is an excellent way of gaining valuable experience across a broad range of different scientific fields. It has also been great for networking, presenting many opportunities to collaborate with external user groups, many of whom are at the very forefront of their particular subject areas," he says.

The various fields of research that are tackled by the different beamlines has also given Gema Martínez-Criado from ID22 the opportunity to expand her horizons. "Collaborations have encouraged me to get involved in fields of research I never thought I would work in," she explains.

Establishing fruitful collaborations is not the only benefit of working at the ESRF. With scientific output now the benchmark for careers in science, the facility can be a great place to build an impressive CV. "The ESRF provides plenty of opportunities to publish, whether it's in the form of collaborations with external groups or novel experiments instigated through your own initiative," Davies explains. In his case, the numbers speak for themselves, with around 45 papers published in the last four years, 17 of which he published as first author.

Unlike Davies and Martínez-Criado, Michela Brunelli recently left the ESRF and is now working at the neighbouring Institut Laue Langevin. For her, it has been a particularly long journey, because she started her PhD at the ESRF before progressing to postdoctoral and then scientist positions. "My new job is similar to my previous one. One reason for this is because I do enjoy the 'service' aspect of it. The other reason is that the technical skills developed at the ESRF are specific for this kind of job," she says.

Looking back, Brunelli thinks that being in contact with top-level material scientists was an important aspect of her experience. She and Martínez-Criado also agree that the freedom to travel to conferences allows for intensive networking in their field of research. In this sense, Martínez-Criado acknowledges that she has been able to start working with German groups from Göttingen that she met at conferences.

Would a scientist recommend the job? For Martínez-Criado the appeal comes from the practical experience on latest synchrotron developments, and the high degree of specialisation of its multidisciplinary staff. "Based on 20 years of experience, the expertise of the beamline staff and associated support engineers provides a solid background to respond to highly demanding problems and needs in a dynamic atmosphere," she says.

"You have to be ready to make significant sacrifices for the beamline during experimental periods," explains Davies. "This is compensated by a certain degree of freedom when things are quieter, such as during shutdowns. In my case this gives me the time that I need to follow my own research interests and test software developments."
MC

Movers and shakers

CEO at the Helmholtz Zentrum Berlin
Anke Pyzalla
Anke Pyzalla left the ESRF Applied Materials and Engineering Beam Time Allocation Panel in December 2008 due to the demands of her new position as scientific director and CEO at the Helmholtz Zentrum Berlin, which is also newly formed, from a merger between Berliner Elektronenspeicherring-Gesellschaft für Synchrotron-strahlung and Hahn-Meitner Institut Berlin. She was previously a researcher and director at the Max Planck Institute for Iron Research, and has been a long-term user of the ESRF, using both X-ray diffraction and tomography on several beamlines, including ID15, ID19, ID31 and ROBL. There she has studied, among other things, the relationship between microstructure and deformation in fossil bones, real-life materials and industrial components. A member of numerous councils (and for several years the ESRF user committee), she is also the editor of the journals *Material Science and Engineering A* and *Journal of Applied Crystallography*, and co-editor of *Journal of Synchrotron Radiation*.

Chair of the directorate of the DESY
Helmut Dosch
Helmut Dosch has spent his career working with light sources, having served as a member of the DESY Scientific Council, been vice-chair of ESRF council and sat on the German Council of Science and Humanities to evaluate the European X-ray Laser Project. In light of this experience, he has been appointed as chair of the directorate of DESY and will take up this position in March. Solid-state physicist Dosch started his scientific career at the Institut Laue-Langevin, before moving into using synchrotron radiation to research solid-state interfaces and nanomaterials. Perhaps his most prestigious role to date was his appointment as director of the Max Planck Institute for Metals Research in 1997.

Directors of research at the Diamond Light Source
Dave Stuart and Trevor Rayment
As a structural biologist, Dave Stuart has used synchrotrons as a crucial research tool throughout his working career. As one of the first users of the ESRF, he led teams studying the bluetongue virus, which continues to spread through Europe's cattle herds, and the HIV virus, the destructive impact of which grows daily.
He took up his appointment as Diamond's director of life sciences in April 2008. His co-director of physical sciences, Trevor Rayment, specialises in research into interface phenomena. To facilitate his research he has developed novel methods of X-ray observation, including uses for synchrotron technology that have led to the study of catalysis in action and corrosion processes.

ESRF director of research
Harald Reichert
Harald Reichert has taken over from Francesco Sette as a director of research. He has been a user of synchrotron radiation throughout his career in solid-state physics. Appointed a project leader at the Max Planck Institute for Metals Research in 1997, five years later he became research professor at the Max Planck Institute for Metals Research, where his group developed sophisticated instrumentation for synchrotron light sources, principally the ESRF. Thanks to his installations, scientists can obtain high-resolution diffraction data not only from the surfaces of metals and alloys but also from interfaces deeply buried in samples.

The ESRF (European Synchrotron Radiation Facility) is a multinational research institute, employing 600 staff, located in Grenoble. It is financed by 19 countries and carries out fundamental and applied research with synchrotron (X-ray) light.

The X-ray Imaging Group of the ESRF is now seeking to recruit:

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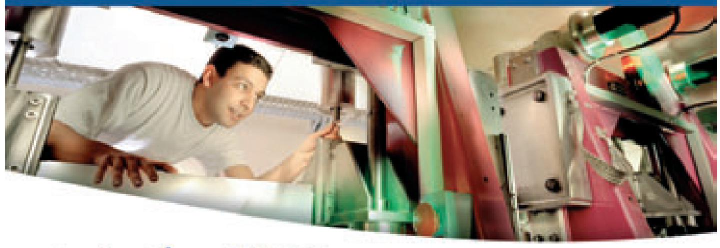
ESRF

A light for science ESRF



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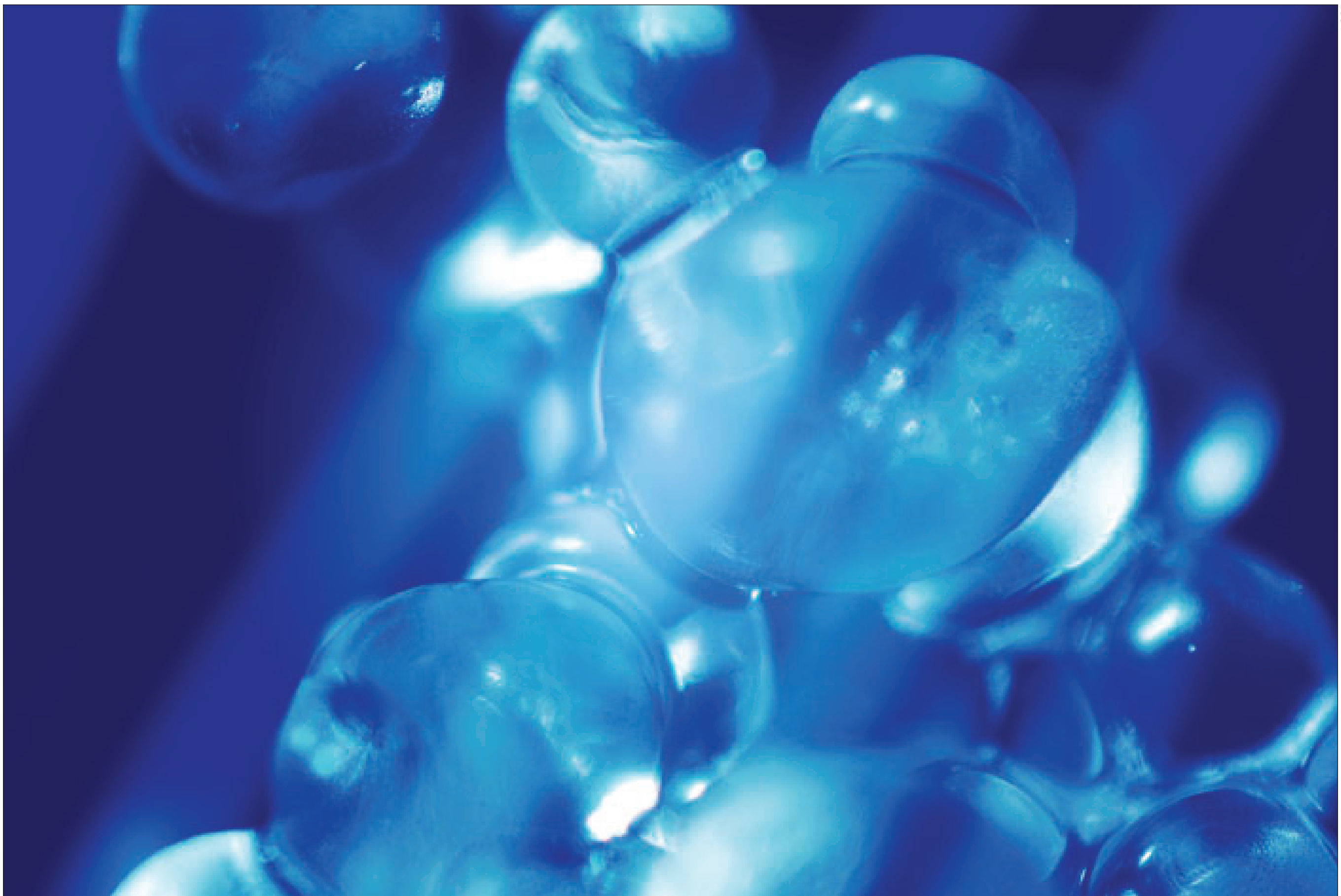


LGGE

Snow White. Under the name 'Snow White', the researchers from this Agence Nationale de la Recherche project create grains of dry snow with the aim of finding out the deformation mechanism of this material. At the ESRF they use the technique of diffraction contrast tomography to determine the form and crystalline orientation of each grain. For more on this subject see p12.

In the corridors

Supporters of synchrotron radiation unite

It seems that synchrotron users and employees are not immune to the social-networking bug – membership of the Facebook group "Supporters of synchrotron radiation" currently stands at 239, with fans from SESAME, Brookhaven, Diamond, the Australian Synchrotron, ESRF and many others. The ESRF is considered to have the best food, even if, as one contributor puts it, "after a while you can calculate the periodic function of the *plat du jour*". Faint-hearted researchers should probably avoid the discussion of "The worst thing you've ever done at or to a beamline", which features horror stories ranging from the prosaic (accidentally hitting the emergency stop and dumping the SPring-8 electron beam) to the nightmarish (a "very expensive fluorescence detector" taking an impromptu shower while its users were having a tea break).

Sci-fi writer hired by the Canadian Light Source

Synchrotrons can seem, to newcomers to the facilities, like places taken from a novel. Despite them being very real, as well as the science they make, the Canadian Light Source (CLS) in Saskatoon will prove that science fiction and reality can merge. The sci-fi author Robert J Sawyer will become a writer in residence at the CLS for the months of June and July, where he will participate in the activities of outreach, mentoring wannabe writers on and off site and working on his own material. Sawyer has written 20 science-fiction novels, of which *Hominids* and *The terminal experiment* have won the Hugo and Nebula awards, respectively. His works are typically set at Canadian science facilities, but so far none have featured synchrotrons – which may change after two months of being immersed in the place.

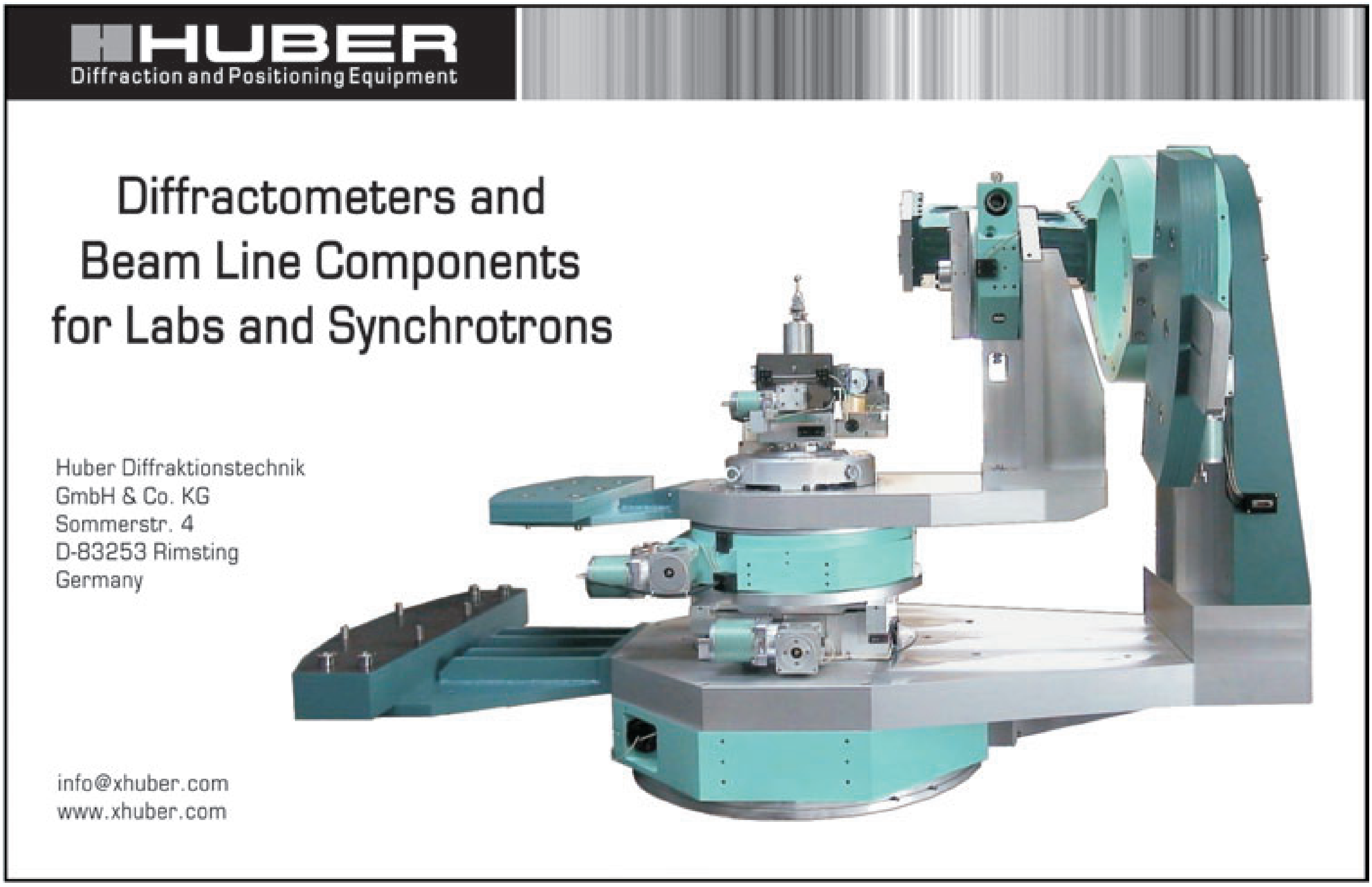
Virtual science pop festival celebrates geek culture

Geekpop is a music festival for that often-neglected subgroup that doesn't want to risk spending a week away from the lab. It "brings together science-inspired artists from around the globe in a gleeful celebration of geek culture". Operating in a fully virtual environment – no litter, queues or ticket touts – Geekpop has full eco-credentials, with its stars arriving via http rather than their personal jets. All of the artists involved, from headliners Amateur Transplants to science writer/rocker Stuart Clark and purveyors of maths-based electro-musings On Rails have agreed to participate free of charge for the tens of thousands of scientifically inclined visitors.

You can visit the Geekpop website to relive last year's festival or to find out more about this year's events.

● **www.geekpop.co.uk.**

GEEK POP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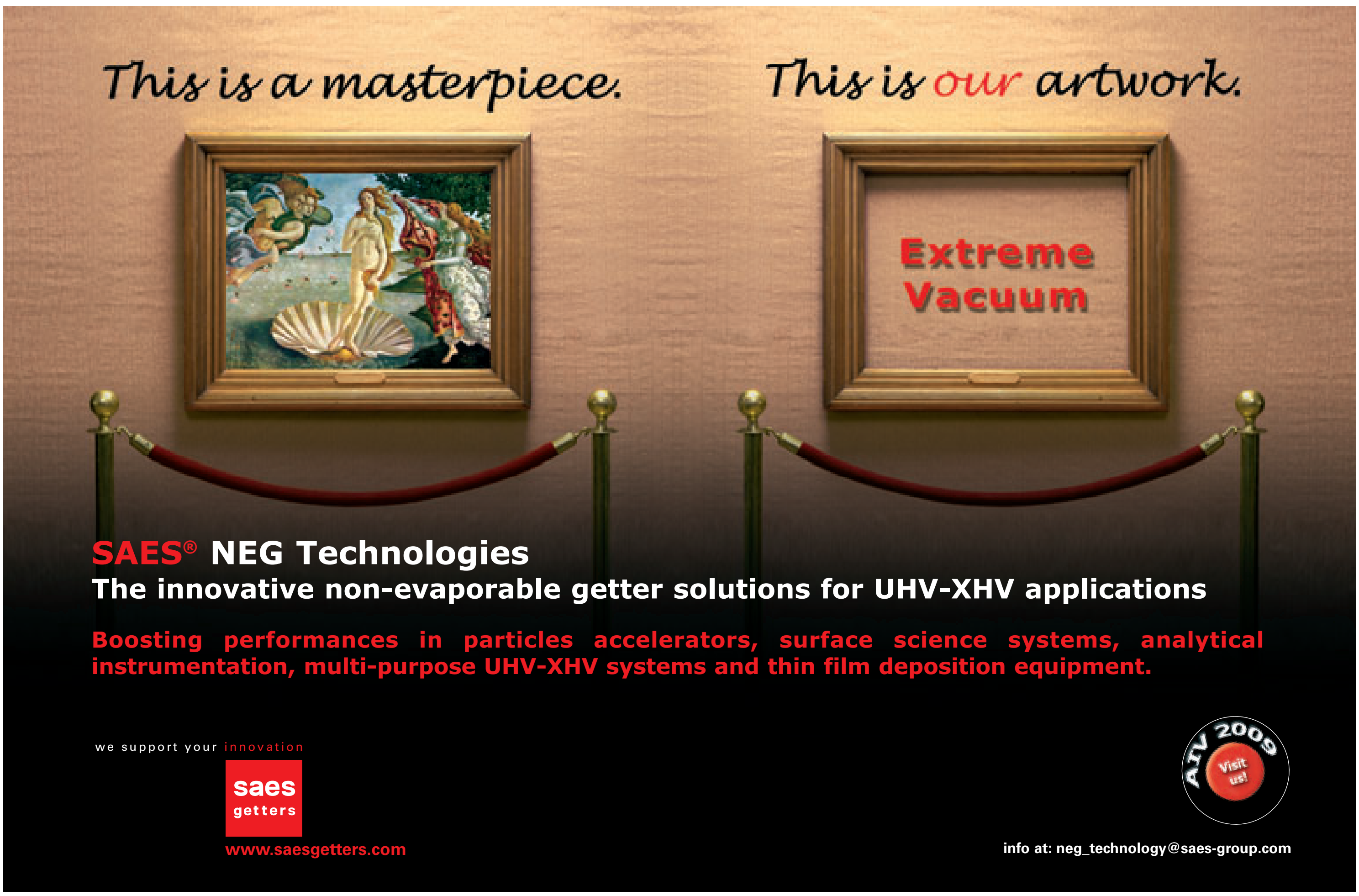
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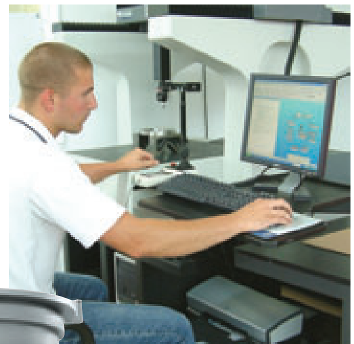

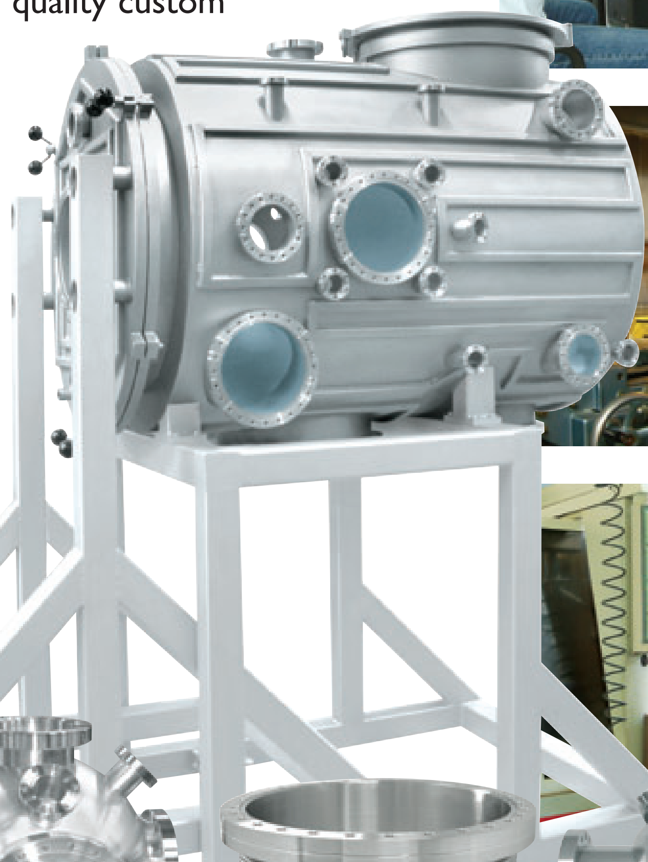

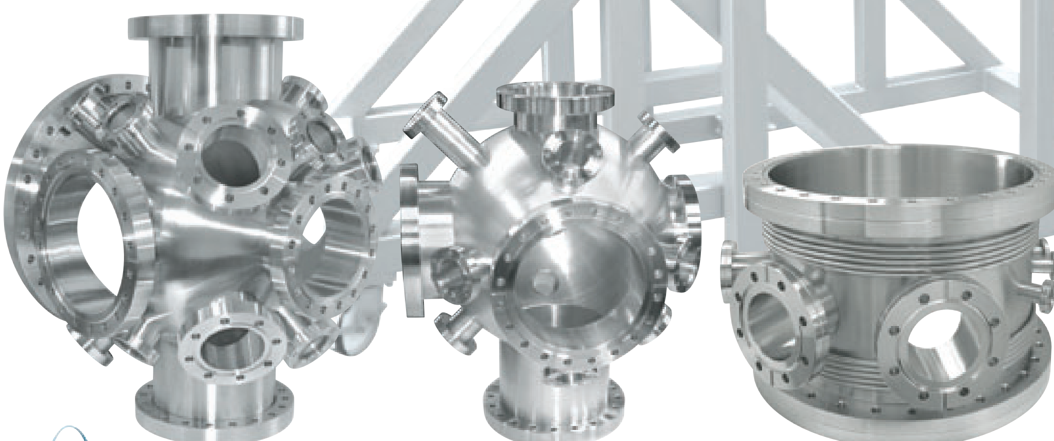

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