A Light for Science

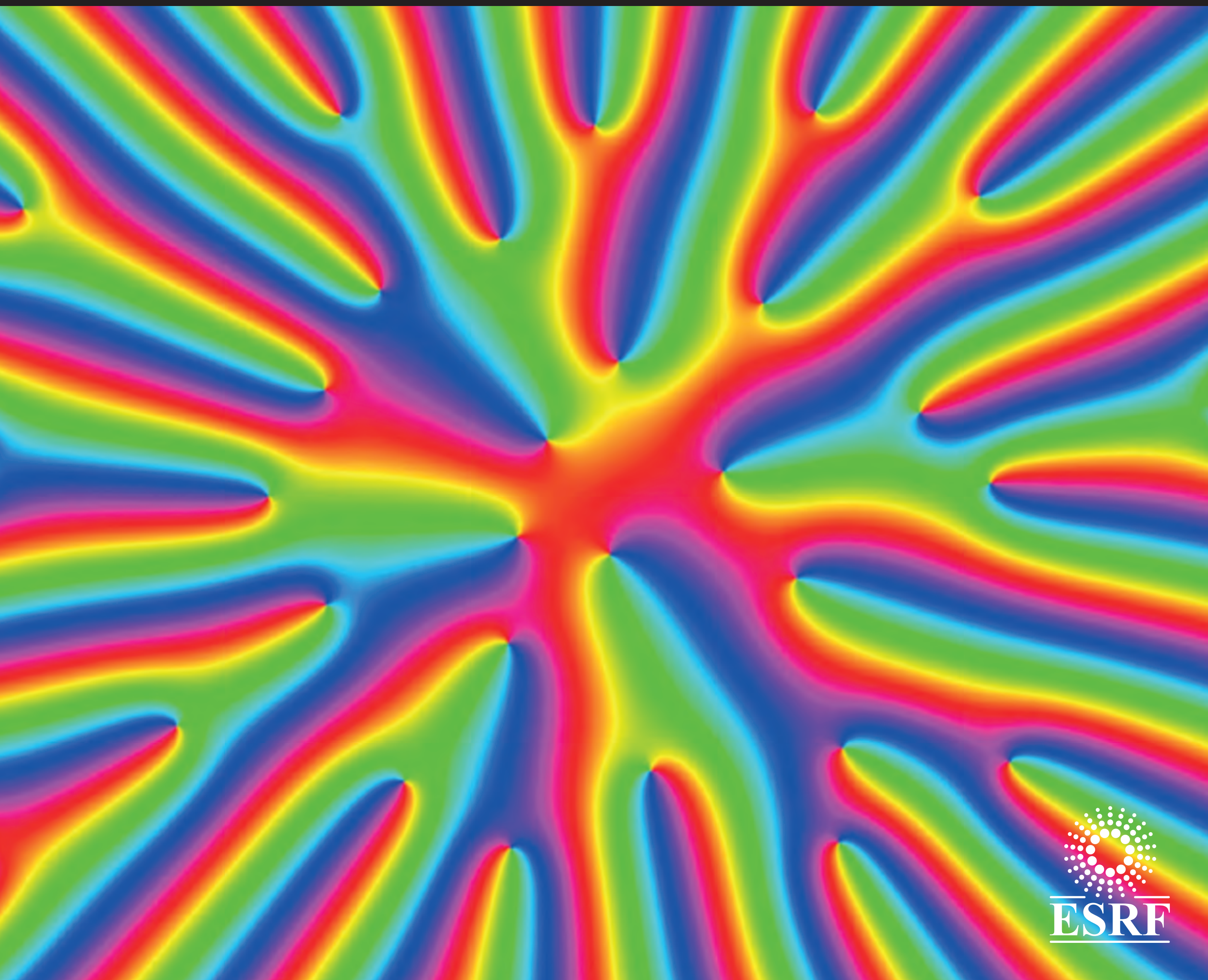
ESRF news

Number 62 December 2012

Physics fundamentals

Towards the ultimate storage ring

Industry success for flu structure



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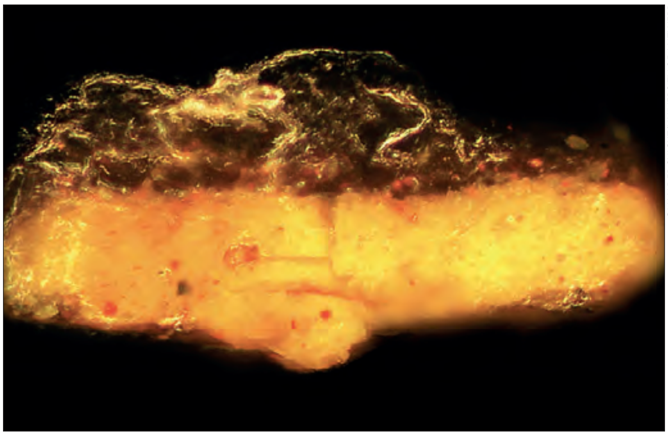
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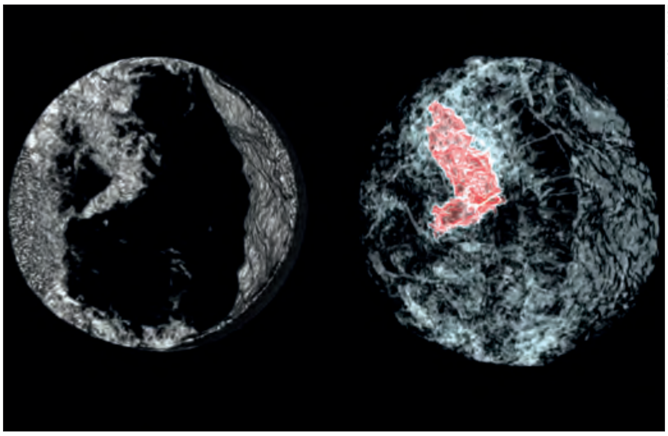
Paint chips from a Van Gogh masterpiece examined at the ESRF, p7.


ESRF/BLASCHA FAUST

Imaging breakthrough for breast cancer, p11.


ESRF/P TAFFOREAU

Crocodile development sheds light on the past, p26.

On the cover:
The phase map of the wave function of a multi-spin quantum system, p19.

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ESRFnews

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Maintaining the balance

The discovery of synchrotron radiation in 1947 is often depicted as a fortuitous observation. In fact, this discovery owes more to research into the mechanisms by which relativistic electrons lose energy that had been carried out in the decades before. As with much fundamental research, theoretical ideas, exploratory experiments and breakthroughs paved the way for the synchrotrons we have today.

Experiments in the early 1960s began to explore the character and potential of this new radiation. Early studies involved measuring the absorption spectra of noble gases, for instance, which led to the discovery of many new phenomena including two-electron excitations. From the start, researchers had pushed to decrease the wavelength of synchrotron radiation from the VUV to soft X-rays, and by the mid-1960s synchrotron radiation had entered the hard X-ray range. This made possible diffraction and spectroscopy investigations of solids, many being basic studies of quantities that today we take for granted, such as absorption cross-sections.

Since then, synchrotron scientists have evolved from being "parasites" of particle accelerators, the pioneers of so-called first generation sources, to dedicated users of second- and third-generation sources in the early 1980s and 1990s, respectively. This has happened in leaps and bounds, and continues to do so with fourth-generation sources and moves towards "ultimate storage ring" sources.

> **"It is doubtful that anyone could have envisaged these developments"**

It is doubtful that anyone in the early days could have envisaged these developments. This is often the case with fundamental research, which has led to new techniques such as EXAFS, magnetic circular dichroism and inelastic X-ray scattering. Bright synchrotron sources have revolutionised X-ray diffraction, imaging and high-pressure research and these, in turn, have impacted planetary science, paleontology, magnetism, physics, chemistry, biology, material science and other fields. Of course, much research carried out at synchrotrons stems from the laboratories of universities and other institutes. But in some cases, for example molecular crystallography, the power of synchrotrons has revolutionised the field.

Nevertheless, it is important for the ESRF to maintain a balance between fundamental "blue sky" experiments and research that is more applied. The constantly evolving user-access model at the ESRF is designed to optimise this balance between fundamental and applied research.

Your views in demand

Phase I of the ESRF Upgrade is a perfect opportunity to push the limits of innovative research, both fundamental and applied. Discussions about Phase II of the Upgrade, which could see the replacement of the storage ring itself, will be held at the 2013 Users' Meeting on 4–6 February to identify the needs of the scientific community in the long term. This could mean transforming the fundamental research of today into applications or initiating research into areas that will set the scene for future breakthroughs. Examples include work on topological insulators that might lead to quantum computers, and basic structural biology research that will undoubtedly lead to new drugs.

Where synchrotron-based research will go in the long term is difficult to say, but there is much to be gained by exploring the limits of temporal and spatial resolution. Exploiting the special characteristics of synchrotron radiation such as its polarisation and coherence, while at the same time using sophisticated sample environments to study matter under all conditions, will help solve some of the most pressing issues faced by modern society. For all this to happen it is mandatory to attract a community that is as broad as possible, be it pure, applied or somewhere in-between.

We are convinced that future progress rests on the fundamental science of today. In this issue of the *ESRFnews* we give a snapshot of some of the fundamental physics research being carried out. It is by no means all encompassing, and it does not cover the painstaking but less high-profile basic research that often underlies new scientific results. But hopefully it will serve as a prompt for discussions about how we should balance our research in the coming decades.

Nick Brookes, *head of the ESRF's electronic structure and magnetism group*

M BANKS

SESAME storage ring takes shape.

Light-source link up

The ESRF and SESAME, the international third-generation light source being built in Jordan, are to benefit from increased co-operation following a visit to the ESRF on 28 September by a SESAME delegation. "Experts coming to SESAME for training and consultation are foreseen and are of great importance," SESAME's technical director Erhard Huttel told *ESRFnews*. "We are very glad to have had equipment from the [German CRG] ROBL beamline and further donations are welcomed."

SESAME is due to switch on in 2016 and its financial situation is in good shape, according to Huttel. "Four member states – Jordan, Turkey, Israel and Iran – have committed to contribute \$1.25 m each for the next four years, and CERN and the European Union will purchase the complete magnet-system and power supplies for the storage ring," he said. "This will allow us to get the storage ring running, although additional means are still needed to get the beamlines operational."

User heads for Stockholm

ESRF user Brian Kobilka of Stanford University has shared the 2012 Nobel Prize for Chemistry with his former mentor Robert Lefkowitz of Duke University, both in the US, for their studies of G protein-coupled receptors (GPCRs) – tiny proteins embedded in cellular membranes that allow our cells to communicate.

The ESRF has made a key contribution to GPCR structures, which offer important new approaches to drug development, because it was the first synchrotron to offer micro-focus X-ray beams.

A key result leading up to Kobilka and Lefkowitz's SEK 8 m award was obtained at the ESRF in 2007, when Kobilka and colleagues solved the first GPCR that binds to hormones or neurotransmitters. Using the ESRF's ID13 and ID23-2 beamlines, Kobilka's group, in collaboration with Gebhard Schertler and colleagues at the MRC Laboratory of Molecular Biology (LMB) in Cambridge, UK, determined the structure of the beta-two adrenergic receptor, β_2AR. "I have a very fond memory of the ESRF," Kobilka told *ESRFnews* last year.

Schertler, who is now at the Paul Scherrer Institute in Switzerland, says several others were in the running for the Nobel prize. "In the end it was awarded for the adrenergic receptor, rather than for pioneering GPCR structure studies, so the award is very well deserved," he told *ESRFnews*. "Of course it would be wonderful if I had got the prize, but Brian Kobilka is a great collaborator, and in a way I am glad not to have the burden that the Nobel prize can bring."

The ESRF results paved the way to Kobilka's next seminal achievement in 2011, obtained using the Advanced Photon Source near Chicago. Here, his team captured an image of the β_2 receptor activating a G protein, which is the key event in how a hormone binding to the outside of a cell eventually causes chemical changes within the cell.

"The thing that sets Brian apart from the rest of us is the beautiful structure of the β_2 receptor bound to a G protein and his work in developing GPCR-T4 lysozyme fusions," says Chris Tate of the LMB, who has made similar breakthroughs in understanding the sister structure β_1AR using the ESRF, also in collaboration with Schertler. "His prize is richly deserved and it is also a fantastic recognition for the whole of the field, because there are hundreds more GPCR structures to be determined."

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Brian Kobilka in the limelight after the Nobel prize announcement.

Users' corner

New system success

The last proposal submission deadline on 1 September saw 956 new proposals received and reviewed during the Beam Time Allocation Panel (BTAP) meetings on 25 and 26 October. This was the second highest number of proposals ever received for a September deadline, despite fewer beamlines being operational due to ESRF upgrade activity. This was also the first time that the new beamline-based committee structure was in place, and was the first test of new software tools designed to handle proposal submissions. The next deadline for submission of standard proposals will be on 1 March 2013, while the deadline for long-term proposals is 15 January 2013.

2013 Users' Meeting

The plenary session of the 23rd ESRF Users' Meeting will take place on 5–6 February. Five workshops dedicated to Phase II of the ESRF Upgrade Programme, which is centered around a potential major increase in the brilliance of the ESRF source, will take place on Monday 4 February with the following themes: X-ray cinematography, structural biology, materials and chemistry, functional soft matter and science at extreme conditions.

More details of the workshops and the ESRF's plans to upgrade the storage-ring lattice can be found on pp8–9, and all users are encouraged to participate to help shape the ESRF's Phase II scientific portfolio. See www.esrf.eu.

News from the beamlines

- **ID02** will be closed for upgrade purposes for approximately nine months beginning summer 2013. The upgraded beamline ID02 is expected to be available in late spring or summer 2014.
- During the scheduling period 2013–II (for which the proposal deadline is March 2013) there will be no beam time available on **ID08**, which will close at the end of July 2013. It will be replaced by an upgrade beamline at position ID32. The branch for soft X-ray dichroism (XMCD) studies on ID32 is planned to be open for users in the first half of 2014 (proposal deadline September 2013). The high-resolution soft X-ray resonant inelastic X-ray scattering (RIXS) branch will open later.
- **ID17** has recently completed a refurbishment of the double Laue Si(111) monochromator, which allows users to select energies in the 25–160 keV range – more than doubling its working range.
- The funding for the XMaS beamline (**BM28**) has been renewed for the period 2012–2017 as a mid-range facility by the UK's Engineering and Physical Sciences Research Council.
- The **BM29** bio-SAXS beamline (formerly ID14-3) has been in successful user operation since June 2012. The commissioning of the new HPLC system (liquid chromatography *in situ*, to be used in parallel with the sample changer robot) is underway and the device will be available for users from spring 2013.

Addressing the SRI audience.

Instrumentation takes centre stage

More than 1000 participants, 650 posters and 72 exhibitors. These are just a few of the striking statistics to have emerged from the 11th International Conference on Synchrotron Radiation Instrumentation (SRI) held in Lyon this July, which was organised jointly by the ESRF and Synchrotron SOLEIL.

"SRI2012 has exemplified both the healthy competition as well as the many collaborative projects between facilities and new photon sources of all kind," concluded scientific co-ordinators Paul Dumas of SOLEIL and Jean Susini of the ESRF. "A real scientific synergy is clearly emerging. Furthermore, the quality and size of the commercial exhibition have reinforced our belief in the growing importance of the partnership between synchrotron facilities and industry."

Delegates from France and Germany comprised 25% and 22% of attendees, respectively, at the four-day event, followed by the US (15%), Japan (14%) and the UK (7%). At 11.2%, ESRF staff made up the largest contribution from a single institute, followed by SOLEIL (8.3%), DESY (6.9%), Diamond Light Source (5.4%) and the Paul Scherrer Institute (4.6%). The bulk of participants were aged 31–50, according to conference organisers.

Scientific proceedings spanned 21 parallel and four plenary sessions, and included four keynote lectures covering the life sciences, industry, environmental science and X-ray free-electron lasers. A group of 270 delegates also took a guided visit of the ESRF.

"This conference confirmed the tremendous progress made by the synchrotron radiation community in many scientific and technical areas over the past few decades," said Susini. "We broke a record for attendance, reflecting the growing size of the community."

The next SRI conference will be organised by BNL/NSLS-II in 2015.

Cultural science continues to bloom

Despite acting with the best of intentions, conservators do not always get things right when trying to preserve famous works of art for future generations. A case in point is the application of a supposedly protective varnish to paintings by Vincent Van Gogh. The Dutch master rarely varnished his works, preferring a vibrant matt finish, but in the early part of the 20th century many of his paintings were coated with varnish that, over time, appears to have had a detrimental effect on the underlying pigments.

Some of the bright yellow flowers depicted in Van Gogh's 1887 oil painting "Flowers in a blue vase", today the property of the Kröller-Müller Museum in the Netherlands, have turned an orange–grey colour. Now, studies performed at the ESRF beamline ID21 and at DESY in Hamburg have revealed why: a hitherto unknown degradation process taking place at the interface between paint and varnish, which causes an unusual grey crust to form in regions that contain cadmium yellow paint.

Researchers already knew that in unvarnished paintings cadmium yellow pigment (cadmium sulphide) oxidizes with air to produce cadmium sulphate, making the pigments lose colour and vibrancy. But instead of an expected slightly off-white oxidation layer, the pigments in this Van Gogh were covered

KRÖLLER-MÜLLER MUSEUM

X-rays reveal the mechanism causing discolouration in the top right-hand corner of Van Gogh's "Flowers in a blue vase".

with a dark, cracked crust. "This intrigued us very much," says Koen Janssens of the University of Antwerp, who led the new study.

To identify what had happened, Janssens and colleagues subjected two microscopic paint samples taken from the original painting to X-ray spectral analysis at the ESRF and DESY, revealing the chemical composition and internal structure at the paint–varnish interface. To their surprise, the researchers did not find the crystalline cadmium-sulphate compounds that should have formed during the oxidation process. Rather, it emerged that the sulphate anions had found a suitable reaction partner in lead ions from the varnish and had formed anglesite – an opaque compound found throughout the varnish.

"At the interface between paint and varnish, the cadmium ions together with degradation products from the varnish itself also formed a layer of cadmium oxalate," says the ESRF's Marine Cotte. Together with the anglesite, the cadmium oxalate accounts for the opaque, orange–grey crust disfiguring parts of the painting on a macroscopic level.

The discovery will force conservators in many museums to readdress the issue of restoring Van Gogh paintings. "This study on the deterioration of cadmium yellow is an excellent example of how collaboration between scientists and conservators can help to improve our understanding of the condition of Van Gogh's paintings and lead to better preservation of his works," says conservator Ella Hendriks of the Van Gogh Museum in Amsterdam, who did not take part in the study. "Many of Van Gogh's French period paintings have been inappropriately varnished in the past, and removal of these non-original varnish layers is one of the challenges facing conservators on a worldwide basis today."

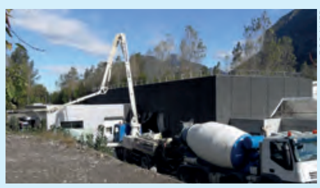
Reference

G van der Snickt *et al.* 2012 *Analytical Chemistry*; DOI: 10.1021/ac3015627.

Towards the world's smallest X-ray beams

A ceremony at the ESRF on 18 October marked the inauguration of the satellite building for the nanoscience beamlines ID16A and ID16B – the first major component of the ESRF upgrade "EX2" construction works to be delivered. The final phase of construction took place in late September with the successful pouring of almost 500 tons of concrete to create the top 35 cm-thick layer of the building's floor.

Due to open for user operation in early 2014, ID16 will offer the world's smallest beams (10–20 nm) for carrying



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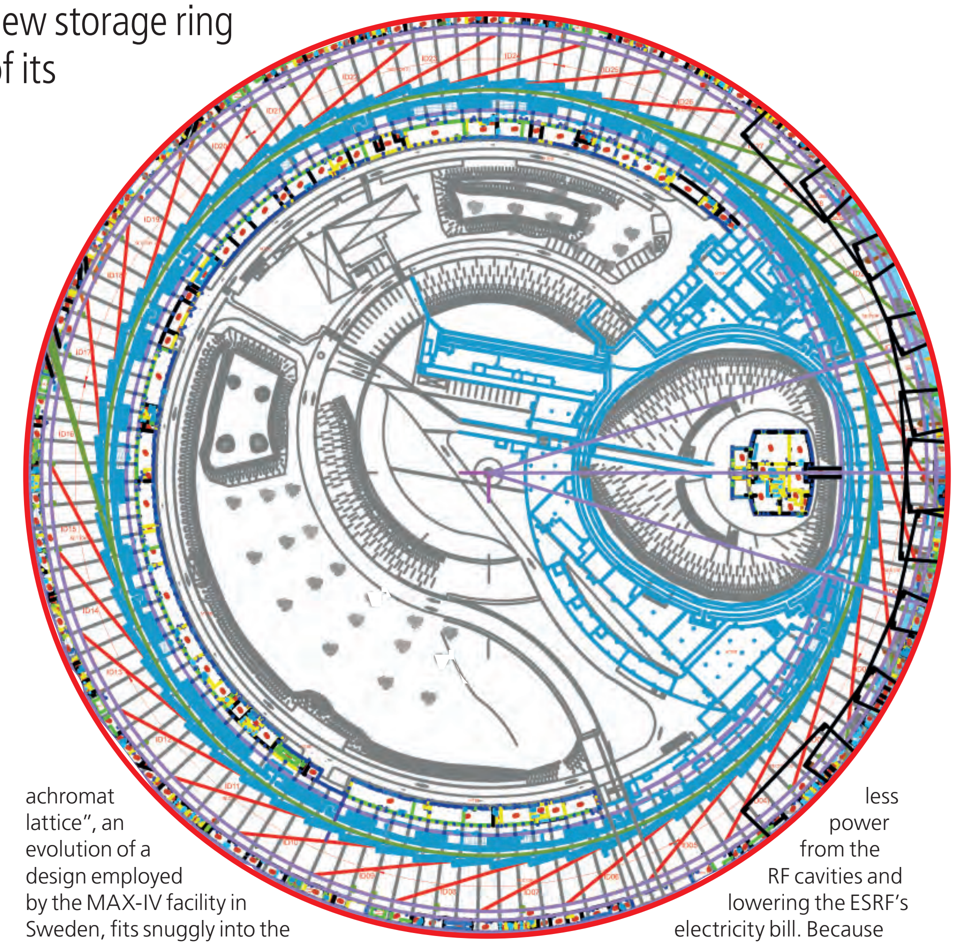
out X-ray nanoscience. Environmental stability is therefore vital, and initial measurements performed by the Technical Infrastructure Division show promising results. "The concrete slab shows very good behaviour in the way that it is curing, and the vibration levels are very small," says scientist-in-charge Peter Cloetens. "The building's temperature control is also working very well."

Once the slab has cured (which takes at least one month) the lead hutches and other heavy equipment can be installed. Following this and various infrastructure work, the beamlines are due to be commissioned in September 2013. "Although the ID16 satellite building is not a prototype for the main EX2 experimental hall extensions, it demonstrates that we can expect excellent performance for the upgrade beamlines overall," says Cloetens.

Supercharging the source

The ESRF unveils plans for a new storage ring that will boost the brilliance of its X-rays by a factor of 50.



Underpinning the ESRF's success is the reliability and high performance of its accelerator complex. Despite major improvements that have given users smaller, more brilliant X-ray beams, the basic magnetic configuration or "lattice layout" of the machine has remained relatively unchanged for the past 20 years. Now, the ESRF is drawing up plans that would see all 32 curved sections of the storage ring replaced with an entirely different magnetic lattice by the end of the decade. If approved, the new machine will boost the brilliance and thus coherence of its X-rays to unprecedented levels, benefitting users across all beamlines, and be the centerpiece of Phase II of the ESRF upgrade.

The first phase of the ESRF upgrade has already seen big changes to the source. A fast beam-position diagnostics system that provides greater electron stability has delivered record values of vertical emittance (less than 4 pm-rad). Emittance is the product of the electron beam's cross-section and divergence, so a lower emittance equates directly to a higher brilliance. Thanks to increased space made available in the straight sections of the storage ring, longer and more powerful undulators can be installed, plus additional undulators are being inserted in canted sections. Finally, radio-frequency (RF) power sources based on semiconductor technology are gradually replacing klystron-based transmitters, while improved RF cavities to be installed on the storage ring during 2013 will be vital to stabilise the shorter bunch length of electrons in the Phase II machine.

A new machine

But many users have long desired a reduction in the horizontal beam emittance, too, which would increase the brilliance even further. The horizontal emittance is the last major machine parameter to be optimised. Changes to the storage ring optics soon after the ESRF started up reduced it from 7 nm-rad to 4 nm-rad, but taking this down further was thought impractical without increasing the size of the storage ring or changing vital infrastructure such as the injector.

Thanks to better magnets and vacuum technologies, and a worldwide effort to develop an "ultimate storage ring", staff in the Accelerator and Source Division have devised a suitable lattice structure that leaves the straight sections of the storage ring intact while only requiring the curved sections to be rebuilt with new components. The new "hybrid 7-bend arc achromat lattice", an evolution of a design employed by the MAX-IV facility in Sweden, fits snuggly into the existing facility.

Rather than using two dipole bending magnets in each arc, as is presently the case, it will pack seven interspersed with strong quadrupoles, thus decreasing the degradation in emittance caused by bending. The new lattice should reduce the horizontal emittance to below 150 pm-rad – 30 times smaller than at present, increasing the brightness of the photon beam by roughly the same amount. For X-ray energies larger than 50 keV, the increase will be even higher. "This is a completely different lattice that will open new fields of scientific exploration," says manager of the ESRF operations group, Jean-Luc Revol. "Up until now there has been an evolution of the machine, but this is a step-change."

Besides its lower emittance, the new lattice will also reduce the energy loss per electron per turn from 5 MeV to about 3 MeV, requiring less power from the RF cavities and lowering the ESRF's electricity bill. Because the lifetime of the beam in the new configuration will be shorter, the Phase II machine will be operated in "top-up" mode.

"It's a completely different lattice configuration."

The technical aspects of the proposal, outlined in detail in a white paper submitted to the ESRF Council at the end of November, are challenging. The ESRF's plans are based on pushing existing technologies to their limits, but R&D will also be undertaken into permanent-magnet design, high gradient quadrupoles and low conductance vacuum chambers to ensure the brightest, most efficient source possible.

The overall cost of the new machine is expected to be around €100 m, with an additional €50 m needed to complete four new Phase II beamlines. Upon approval of the white paper, the ESRF will embark on a technical design study. Should the green light be given, the machine will be stopped for approximately one year from August 2018 to dismount, reconstruct and commission equipment in the tunnel, with beam becoming available for users in late 2019.

Other light sources, notably SPring-8 and the APS, are planning similar upgrades in brilliance, says director of the Accelerator and Source Division, Pantaleo Raimondi. "With this upgrade, the ESRF will be less than a factor of 10 away from the ultimate limit in emittance, when the source becomes diffraction limited," he says. "If it goes ahead then we are going to be the brightest source in the world."

Boosting the beamlines

The ESRF's new storage-ring lattice would produce more brilliant and thus more coherent X-rays with characteristics approaching those of a laser, increasing the amount of structural information that can be extracted from a sample. In addition to the new lattice, Phase II of the ESRF upgrade will see four new beamlines extending into the Chartreuse and Vercors building extensions.

The existing beamline portfolio will need to be adapted in order to benefit fully from the performance of the new source, mostly involving moderate upgrades to mirror systems and crystal monochromators. "Phase II of the ESRF upgrade is catering for a similar performance-increase of the X-ray source as will be achieved during Phase I for the beamline portfolio," states research director Harald Reichert. "The benefit for the scientific community will be immediate and enable experiments on soft and hard condensed matter with unprecedented performance."

Matthew Chalmers

Exploring the potential of an ultimate storage ring

Five workshops will be held in conjunction with the next users' meeting on 4 February 2013 to explore the scientific opportunities on offer from Phase II of the ESRF upgrade.

- **From functional soft matter to biology: future challenges**
  To fully exploit the outstanding properties of the upgraded source, new scattering and diffraction methods will be required. One challenge is to design experiments that allow radiation sensitive systems to be investigated with the enhanced brightness, as well as identifying new problems that cannot be addressed with existing facilities.

- **X-ray cinematography with the new coherent source**
  A drastic increase in photon flux at the sample position will benefit all imaging techniques, and extend synchrotron-based imaging to much shorter time-resolved X-ray imaging covering fields including materials science, soft matter and biology, microelectronics, biomedical imaging, environmental science and chemistry.

- **Seeing is believing: the future of structural biology**
  The new storage ring will dramatically change the way in which structural biology is carried out, requiring diffraction data to be extracted in a matter of milliseconds. The combination of small beams, high flux and greatly increased coherence will also provide opportunities for research not previously considered.

- **Phase II prospects for materials and chemistry**
  Increased brightness and coherence will benefit experiments exploiting the coherent properties of the beam and/or requiring very high spatial resolution, such as coherent diffraction imaging, *in situ* studies of catalysis and metallurgy.

- **Science at extreme conditions with an ultimate source**
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Cancer-screening synchrotron style

A new technique honed at the ESRF allows precise imaging of the breast with a radiation dose much lower than existing clinical methods.


ESRF/BLASCHA FAUST

Paola Coan, Alberto Bravin and Emmanuel Brun at the ESRF surveying images of a breast sample obtained by conventional (left) and phase-contrast X-ray imaging (right).

Screening to detect early signs of breast cancer, which affects nearly one in eight women in their lives, is common practice in many countries. But whether screening does more harm than good is a matter of debate. A review published in the *Lancet* medical journal in late October showed that screening saved around 1300 lives every year in the UK, but led to some 4000 women having treatment for cancers which, if ignored, would never have caused a problem during a woman's lifetime.

One of the main causes of unnecessary treatments, which can involve surgery or radiotherapy, is the lack of specificity of diagnoses possible with present clinical equipment. Computed tomography (CT), a powerful X-ray technique that produces precise 3D images of human tissue, cannot be routinely applied to diagnose breast cancer because very high doses are required to discriminate between normal and cancerous tissue. Instead, screening typically employs dual-view mammography, in which low-energy X-rays produce two images of the breast. However, 10–20% of breast tumours are not detectable on mammograms and the technique also leads to a large number of false–positive diagnoses. "This is a big health issue involving millions of women worldwide," says the ESRF's Alberto Bravin.

Higher resolution, lower dose

To overcome these limitations, Bravin and Emmanuel Brun at the ESRF, along with Paola Coan and colleagues at Ludwig Maximilians University in Munich (LMU) and physicist John Miao and his team at the University of California int Los Angeles (UCLA), have developed a way to produce high-resolution 3D images of the breast using doses 25 times lower than conventional CT scans. Unlike conventional imaging, which relies on detecting changes in the absorption of X-rays as they pass through different tissue types, the technique uses phase-contrast imaging (*PNAS* **109** 18290 2012).

Developed at the ESRF and elsewhere in the late 1990s, phase contrast imaging exploits the refraction of X-rays, which is much more sensitive to differences in tissue composition than conventional absorption-based X-ray imaging. The ESRF and the LMU teams combined the technique with high-energy X-rays, which are absorbed by the tissue, and a novel CT reconstruction algorithm developed by researchers at UCLA to image in 3D a whole human breast with a higher resolution than ever before, while delivering a dose deemed safe by radiation protection standards.

"It is the first time that this has been done," says Coan. Now, she explains, the team has to work out how to replicate the high-energy, monochromatic, almost parallel X-ray beams provided by a synchrotron in a clinical setting. "You can't put a synchrotron into a hospital, at least not as we know it."

Compact synchrotron sources

As welcoming as third-generation synchrotrons might be, they are hardly ideal settings in which to host large numbers of patients, although the ESRF's ID17 beamline does boast clinical facilities and in the past has hosted coronary-angiography clinical trials in about 60 patients (see box).

One alternative is to develop compact synchrotron sources – room-sized devices that generate X-rays via "inverse Compton scattering", rather than by the deviation of electrons circulating in a storage ring. Costing less than €10 m, explains Bravin, such sources would be relatively cheap and there are various compact sources under development in Europe. These include "ThomX" at the Laboratoire de l'Accélérateur Linéaire in Orsay, France, scheduled to be operational in 2016 and which also the ESRF is involved with, and one at the Centre for Advanced Laser Applications in Garching, Germany.

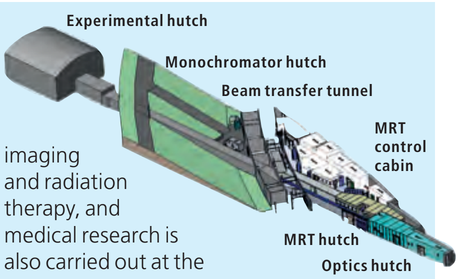
The other way to take phase-contrast imaging out of the lab is to convince large companies who already produce X-ray sources of the potential of the new technique. "We need more powerful X-ray sources to do what we can do now in a clinically compatible time," says Bravin. "With existing sources you need many minutes of exposure, which is far too long to expect a patient to remain still."

Matthew Chalmers

The ESRF's clinical dimension

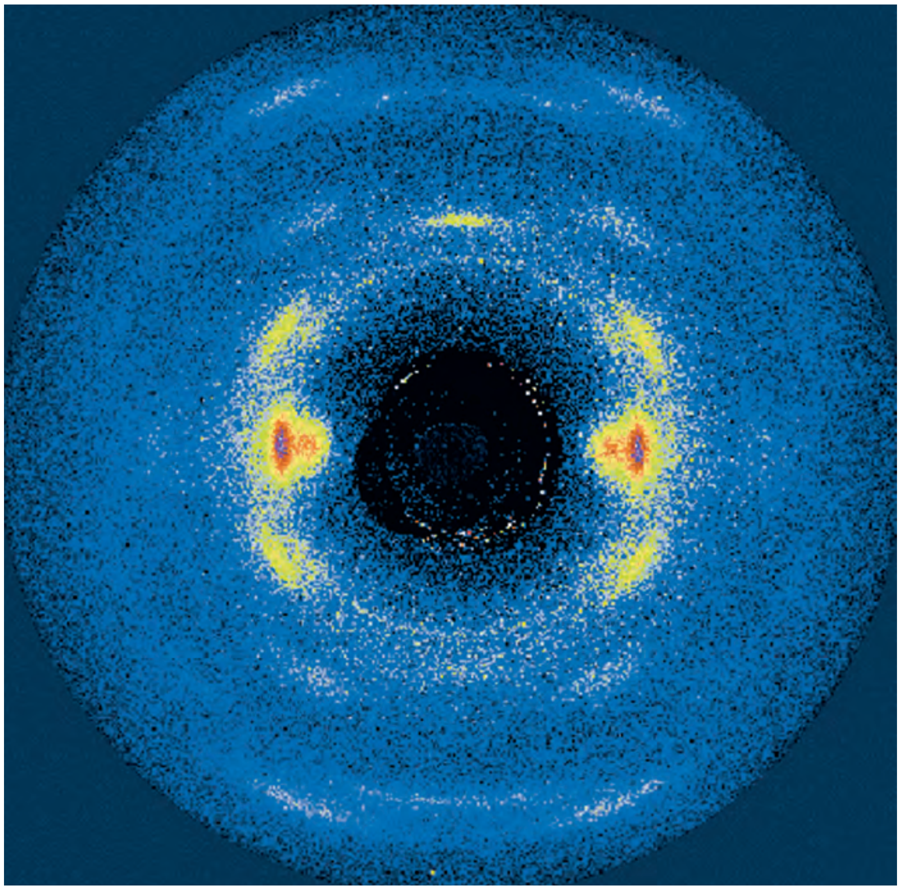
The ESRF's ID17 beamline is one of around five in the world dedicated to medical applications. It specialises in preclinical and clinically oriented medical research undertaken by users working in biomedical imaging, radiobiology, microbeam radiation therapy (MRT) and radiosurgery, and ID17 staff have developed strong relations with European hospitals.

Cell and molecular laboratories at the beamline allow sample preparation and early follow-up after irradiation, while preclinical housing and surgery facilities, along with a histology room, complete the ESRF's Biomedical Facility. ID17 is also used for fossil imaging and radiation therapy, and medical research is also carried out at the ESRF's ID19, ID21 and ID22 beamlines. "We are at the forefront in medical research with synchrotrons, both in imaging and therapy," says scientist-in-charge Alberto Bravin. "Thanks to excellent instrumentation and a skilled team we are probably the world reference in our field."



Expect the unexpected

Publicly funded research is increasingly expected to produce near-term returns to society. Fundamental physics has a strong track record of doing just that.



JOURNAL OF APPLIED CRYSTALLOGRAPHY **30** 390

The discovery of X-ray crystal diffraction in 1912 opened a new view on material structure, as this diffraction pattern from a single silk fibre illustrates.

It is 100 years since physicist Max von Laue discovered that X-rays are diffracted by a crystal. Soon after his demonstration, William Bragg and his son Lawrence derived a formula that connects the X-ray diffraction pattern to the crystal's 3D atomic structure – the cornerstone of experiments at the ESRF's beamlines. Einstein rated the discovery of X-ray diffraction in crystals one of the most beautiful in the history of physics.

These pioneers of X-ray crystallography did not set out to find a technique that would revolutionise materials science, drug design, palaeontology and numerous other disciplines. They were simply trying to better understand the properties of X-rays, which had been discovered serendipitously 15 years earlier.

"There seems to be a general fear these days that fundamental physics should be apologised for, but I think that we should be bold about it," says Peter Knight, president of the UK's Institute of Physics (IOP). "We need to protect our heritage and the best way to do so is to tell people what fundamental research has achieved. Sadly, once physics finds something useful, such as electronics, it tends to get rebranded."

Applied or not applied?

Today the ESRF covers studies ranging from the nature of fundamental space–time symmetries to the development of catalytic converters in partnership with industry, but most physics experiments fall between such extremes. "I would say that 80% of what we do here is just motivated by scientific curiosity, but nobody says that because of the present financing structures," remarks José Baruchel, emeritus scientist at the ESRF. "There was a time when you could get funding for pure fundamental topics: the last time I got a European grant for that was in the 1990s."

Applied research is not a very useful term, says ESRF research director Harald Reichert. "We sometimes call it pre-competitive research, where you lay the ground for future technologies. That's the ESRF's strength."

Starting this year, ESRF users are invited to indicate the societal theme in which their research fits, for example energy or health. This, says Reichert, takes into account that science policymakers have to justify to taxpayers why a facility such as the ESRF should be funded. "We are being challenged by the need to evaluate every aspect of our operation so we have to find a good balance between fundamental and applied research," he says. "The emphasis has shifted more towards applications in recent years, which is fine because, in fact, doing industrial research is part of the ESRF's convention, but we must stay open for fundamental research too."

"We're not asking people to predict the output of their research, but to identify potential uses."

Directed research

Knight says that directed research is not necessarily a bad thing, and cites the development of the laser in the US as an example of where government and industry support boosted the pace of invention. But he worries that the EU framework programme, for instance, is "too aligned with the immediate" because managed programmes can often lead to something more mundane than envisaged. Knight offers graphene, the discovery of which earned two UK-based physicists the 2010 Nobel Prize for physics, as a counter example. "Graphene research was funded by Royal Society fellowships that give recipients complete freedom in their research, and look what came from that."

While it is common practice these days for scientists to explain the applications of their research in the opening pages of a grant proposal, rarely do those applications materialise, at least in the near term. Fundamental science is a pre-requisite for applied science, says the ESRF's Michael Krisch. "The discovery of superconductivity was driven by curiosity or perhaps even by accident, but then systematic fundamental research led to the discovery of high-temperature superconductivity and industrial applications followed."

It is important that we reflect on this, says Reichert. "The danger is that with large funding packages being made available for specific goals, say better batteries, everyone does similar experiments and this actually constrains science because it reduces the scope for mavericks. Every so often a crazy proposal will come up with something important, then funding can be directed at it."

Applications out of the blue

Physics is littered with examples of fundamental, curiosity-driven research that has had unforeseen benefits to society: nuclear magnetic resonance and medical scanners; giant-magnetoresistance and hard-drive capacities; quantum mechanics and the transistor; particle physics and the World Wide Web, to name but a few. Of course, much curiosity-driven physics research never leaves the library. The issue facing scientists and funding agencies today is whether breakthroughs can be streamlined by directing public money towards specific goals and applications.

Return to society

David Delpy, an applied physics graduate who is currently chief executive of the UK's Engineering and Physical Sciences Research Council (EPSRC), which funds most of UK researchers' beam time at the ESRF, admits that the demand for societal returns from science is now more explicit than it was 20 years ago. But he rejects claims that science is only now being asked to produce returns. "If you go back to Darwin's voyage or Harrison's chronometer, all were funded for a very specific purpose: to help Britain rule the waves and expand its influence. And then there are figures like Wedgwood who had commercial applications firmly in mind."

Delpy says that the research funded by the EPSRC has consistently favoured "discovery-led" rather than "challenge-led" research over the past 15 years, with 60% of funds currently going to the former. "Funding fundamental science is implicit in EPSRC's function and that's why we have just committed more funds to the ESRF's XMaS beamline," he explains. "We're not asking people to predict the output of their research, but to identify potential areas where it would be useful."

Regardless of whether a physics research programme leads to a technology or product, says Knight, it produces highly numerate graduates who go on to work in industry or set up a company. "Fundamental physics – quantum theory, the Big Bang, astrophysics and synchrotrons too, although they perhaps have more of an image problem – these are the things that get people into science," he told *ESRFnews*. "This is a huge tangible benefit of basic physics research, and one where there are gender issues because research seems to suggest that women are more likely to want to do something that benefits society."

Quoting the late George Porter, a Nobel laureate in chemistry and former president of the Royal Society, Knight says that there is no such thing as non-applied research – only research that is yet to be applied. "When the ESRF does fundamental stuff, it will almost certainly be related to materials under certain circumstances, and bang! An application will come from it that was not expected."

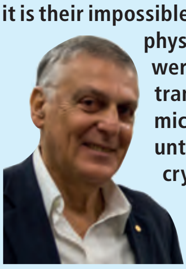
Synchrotrons themselves were a by-product of particle physics – the bluest of blue-skies research into nature's fundamental constituents. In 1969, physicist and founding director of the US laboratory Fermilab, Robert Wilson, was asked by a congressional committee whether Fermilab's new accelerator would have any value for national security. He replied: "it has nothing to do directly with defending our country except to help make it worth defending."

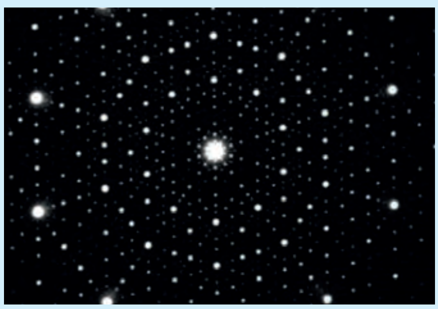
Matthew Chalmers

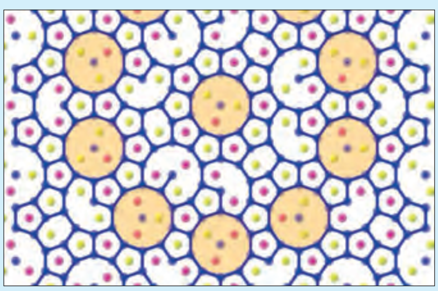
Impossible crystals

For 70 years following the discovery of X-ray crystal diffraction, the textbook definition of a crystal remained unchallenged: a crystal is an ordered, periodic structure. But in 1982, Dan Shechtman (pictured below) at the Technion Israel Institute of Technology rocked the world of crystallography with the discovery of the first ordered but non-periodic crystal: a quasicrystal, which has higher crystal symmetries than are possible in periodic systems. Hundreds of quasiperiodic crystals have since been discovered, and last year, having initially faced strong opposition for his finding, Shechtman won the 2011 Nobel Prize for Chemistry.

Quasicrystals have been used to reinforce steel and polymer composites and even to make non-stick coatings for frying pans. But it is their impossible structure that attracts physicists. Quasicrystals were discovered using transmission electron microscopy, and it wasn't until a few years later that crystals were grown large enough to be studied using X-rays. Since the beginning, explains ESRF user Marc de Boissieu of the CNRS in Grenoble, the ESRF and the ILL have played an active role in understanding quasicrystals. "This has been a long story that led to key results in the understanding of the structure and the dynamics of quasicrystals."







Diffraction pattern (top) and structure of icosahedral quasicrystals.

Diffuse X-ray scattering measurements have been vital in understanding fluctuations specific to quasicrystals called phasons. Another prominent result, says de Boissieu, was a study performed at the French CRG beamline BM02 in 2007, which revealed the structure of the binary cadmium-ytterbium quasicrystal (left, bottom; *Nature Materials* 6 58).

"The high-quality data acquired allowed us to solve, for the first time, the structure of a quasicrystal at a level comparable to what is achieved in standard crystallography," he explains. "This paved the way to the understanding of physical properties of their formation." The Swiss–Norwegian CRG beam-line, meanwhile, has provided a much better understanding of decagonal phases and, more recently, of a soft matter quasicrystal with 12-fold and 18-fold symmetry, while experiments at ID19 have imaged the *in situ* growth of quasicrystals.

On 18–19 October, Shechtman and 20 others met in Grenoble to discuss the state of the art in quasicrystal research. "Whereas the structure of quasicrystals and some of their physical properties are well understood, the mechanisms bringing in the long range quasiperiodic order remains one of the big questions," says de Boissieu.

Pressure turns simpli

High-pressure experiments at the ESRF are rewriting the phase diagrams of the elements, revealing surprising complexity and new material behaviour.

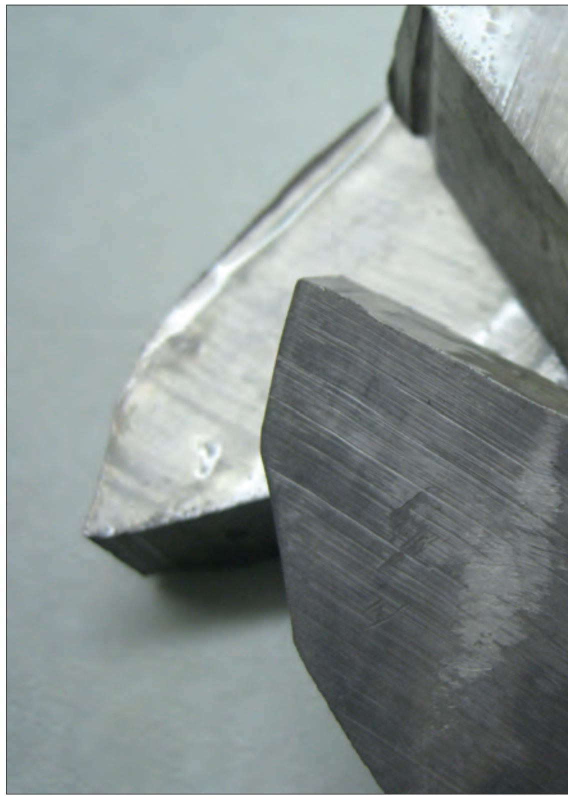
That coal can morph into the hardest and most highly prized structure known, diamond, is a dramatic example of high-pressure physics in action. When an element is subjected to very high pressures, its interatomic distances are reduced and its electronic structure shifts markedly with respect to the same system at ambient conditions. Pressure is therefore a powerful tool to probe the relationship between the structure of materials and their properties.

Advances in synchrotron instrumentation have brought about a renaissance in mapping out the phase diagrams of the simplest systems, such as hydrogen, lithium and sodium. The ESRF provides X-ray diffraction and spectroscopy studies of samples compressed to pressures more than two million times greater than atmospheric pressure using diamond anvil cells, and subjected to temperatures ranging from 5 K, in a cryostat, to 5000 K using lasers.

"There has been great progress during the past 20 years in our understanding the fundamental physics of condensed matter under extreme conditions, thanks in part to third-generation synchrotrons," says Paul Loubeyre of the CEA in Bruyères-le-Châtel, France. Structural, magnetic, dynamic and electronic properties can now be measured with similar accuracy and resolution as if the material were at ambient pressure, he explains, and many old paradigms ruling the high-pressure behaviour of materials have been proven to be not so simple: for instance, the evolution to close packing structures, the breaking of molecular bonds or the systematic evolution to a metallic state. "The reality is indeed richer and more complex than anticipated," he says.

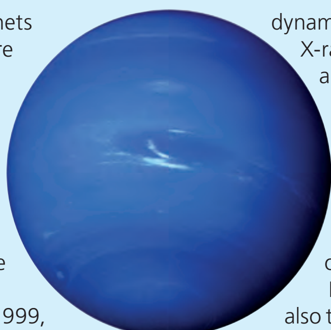
Rich testing ground

The simplicity of hydrogen and the alkali metals makes them a rich testing ground for fundamental physics, since nowadays such systems can be modelled in sufficient detail to allow close comparison between theory and experiment. "The holy grail is to produce metallic hydrogen, and to convincingly prove its existence," explains the ESRF's Michael Krisch.



Sodium, which is a soft metal under ambient conditions, reve

Planetary interiors laid bare



Inside the distant, cold planets Neptune and Uranus, where pressures reach 300 GPa and temperatures top 5000 K, strange phases of water, ammonia and methane ice are predicted to exist. At moderate pressures and temperatures, ammonia ice (NH_3) is a molecular crystal similar to water ice. But in 1999, theorists calculated that ammonia enters a new phase – superionic ammonia ice – under the extreme conditions of planetary interiors. Superionicity is an exotic state of matter that behaves simultaneously as a crystal and as a liquid.

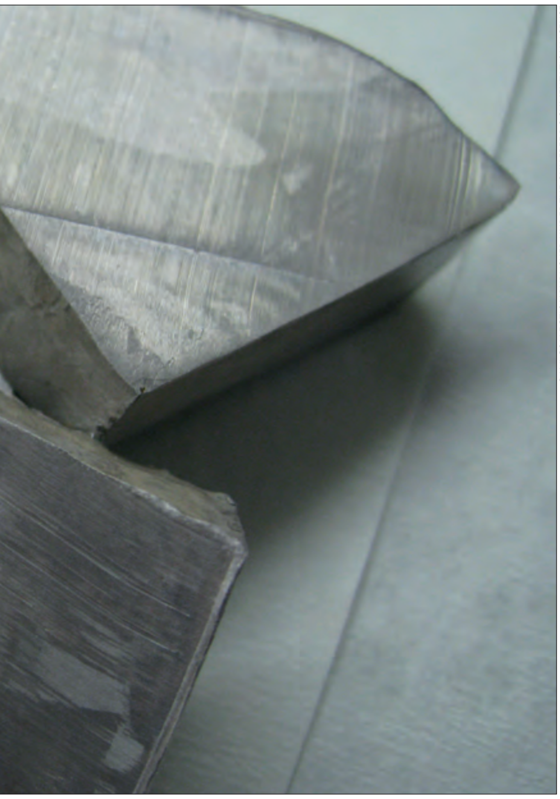
This year, ESRF users from the Université Pierre et Marie Curie in Paris observed the new ammonia state – called the alpha phase – for the first time (*Phys. Rev. Lett.* **108** 165702). It occurred at pressures above 60 GPa and temperatures above 750 K, which is slightly warmer than the molecular dynamics simulations suggest. X-ray diffraction showed that ammonia's nitrogen sub-lattice is the same as in the low temperature solid, but that the hydrogen atoms are much less ordered. Superionic ice that exists inside Neptune and Uranus is suspected to be the origin of their magnetic fields.

Experiments at the ESRF are also tackling our own planet's interior, namely its hot dense iron core. Last year the ID24 beam line was inaugurated, where powerful pulsed lasers will reproduce these extreme environments for a few microseconds at a time. Such setups allow the liquid phase to be explored at pressure, in particular to find out how liquids evolve from a dense molecular state to a plasma. "Warm dense matter plays an important role in stellar interiors and fusion research," says the ESRF's Michael Hanfland. "But it's also a new state of matter that can't be simulated very easily."

Sodium's phases have been the subject of intense scrutiny at the ESRF, and raised several surprises. In 2008, for instance, a study by Eugene Gregoryanz from Edinburgh University, UK, and colleagues unveiled "extraordinary" liquid and solid states of sodium at pressures above 100 GPa that involved seven different crystalline phases (*Science* **320** 1054), while an earlier result by the same group showed a large, pressure-induced drop in sodium's melting point at high pressures (*Phys. Rev. Lett.* **94** 185502). Similar oddities have been found in the lighter alkali metal lithium. Above pressures of 60 GPa, lithium adopts novel crystal structures with up to 88 atoms per unit cell. Both sodium and lithium lose their metallic state under pressure and become semiconductors (*Nature Physics* **7** 211).

Solid oxygen, which is a slightly more complex diatomic molecule, has been turned into a metal at pressures above 96 GPa and, uniquely for a molecular state, becomes a superconductor at very low temperatures. "The structure is vital to know what's going on, and a big surprise has been observed," says Loubeyre: in the solid phase, O_2 molecules associate with pressure to form O_8 entities that ultimately connect to form the metallic state (*Phys. Rev. Lett.* **102** 255503). The other

city into complexity



eals a different side at high pressure.

> **"Essentially we have a new periodic table at pressures of 100 GPa."**

archetypal diatomic molecule, N_2, has a completely different evolution under pressure, he adds: the triple bond is broken and a polymeric phase of single-bonded nitrogen has been observed (*Nature Materials* **3** 558). "Interestingly, recent calculations predict that at pressure in excess of 300 GPa nitrogen will form a new structure with N_{10} that has never been observed."

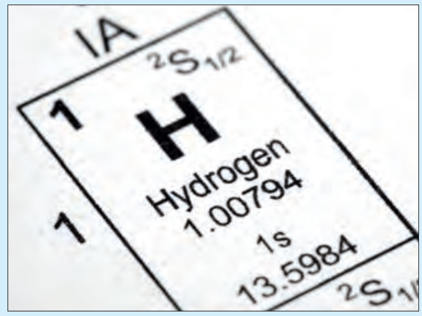
The new periodic table

Essentially, says Loubeyre, researchers have a new periodic table at pressures of 100 GPa, and therefore a new landscape of condensed matter physics to understand. Most of the work so far has been performed on the novel structures adopted by elemental solids at high pressure, but many more surprises remain to be discovered by understanding the new chemical rules of this table so as to synthesise new compounds. One of the key questions to be addressed is whether the properties of elements and compounds apparent at high pressure can be recovered in ambient conditions. "We can call it the emergence of complexity of high pressure," Loubeyre explains. "For example, van der Waals compounds exist only under pressure and are now observed ubiquitously, while many other interesting new compounds are being predicted, such as LiH_6."

With the far corners of the phase diagrams of the simplest elemental solids becoming well explored, researchers are turning to the more complex rare-earth metals: the lanthanides. Cerium surprised ESRF users Frédéric Decremps of the Université Pierre et Marie Curie and co-workers last year, when they subjected a unique single crystal of cerium to a pressure of 0.75 GPa. Unlike most solids under pressure, which undergo a decrease in volume due to changes in their atomic structure, cerium's volume decreased without any accompanying change in its structure. In fact, the team claims that despite the single-crystal nature of the sample the transition is more like the liquid-gas transition of classical systems (*Phys. Rev. Lett.* **106** 65701).

This year, an experiment conducted jointly between the ESRF and users from Edinburgh University put heavier europium, which is divalent rather than trivalent, under pressure (*Phys. Rev. Lett.* **109** 095503). The team uncovered a new phase in the lanthanides – an "incommensurately modulated crystal structure" – in which the atoms are displaced by a small amount from their expected crystal location. The study, says the team, motivates further density-function-theory calculations to uncover the mechanism behind europium's strange high-pressure behaviour, which includes becoming superconductor with a transition temperature of 1.8 K.

The high-pressure periodic table has also gained its first actinide, uranium, which has a complex ground state and becomes a superconductor at pressures of 1.5 GPa. These systems are still a long way away from "real life" materials, but by building up an understanding of the simplest systems researchers hope to shed light on more complex ones. "These things were not possible a few years ago," says the ESRF's Michael Hanfland, "The past 5–10 years has seen the development of ab initio prediction of structures thanks to new efficient algorithms and ever-increasing computing power."
Matthew Chalmers



Towards metallic hydrogen

Even familiar systems can shock physicists when put under pressure. Take the evolution of elemental melting curves and the structural changes in the dense fluid phase. The melting point of iron, for instance, shows discrepancies between theory and measurement at high pressures, which is important for studies of the Earth's interior. Recently, the use of X-ray synchrotron diffraction has been shown to be crucial in obtaining a correct determination of the melting curve, as illustrated in the case of tantalum (*Phys. Rev. Lett.* **104** 255701). Longer term, the aim is to extend the temperature domain in order to bridge the gap between condensed matter physics and plasma physics – a domain called warm dense matter. That will probably require adapting dynamic compression techniques to synchrotrons.

But it is the simplest system of all – hydrogen – that has confounded physicists the most. Hydrogen's metallic phase, predicted since the 1930s, has still not been unambiguously observed. Furthermore, the structural changes of solid hydrogen along its route to metal hydrogen, as measured by single crystal X-ray diffraction at the ESRF, are challenging because they are driven by nuclear quantum effects (e.g. *Nature* **435** 1206). Ultimately, dense hydrogen should create a new form of matter called a quantum liquid that may be both a superconductor and a superfluid near absolute zero, which would be extremely hard to characterise. This year physicists at the Max Planck Institute for Chemistry in Mainz, Germany, claimed to have observed the metallic transition in a diamond anvil cell at 300 K (*Nature* **486** 174), but the jury is still out.

"The precise pressure at which it happens is not known, but metallic hydrogen should exist," says Patrick Bruno, head of the ESRF's theory group. "The discovery would probably be worth a Nobel prize."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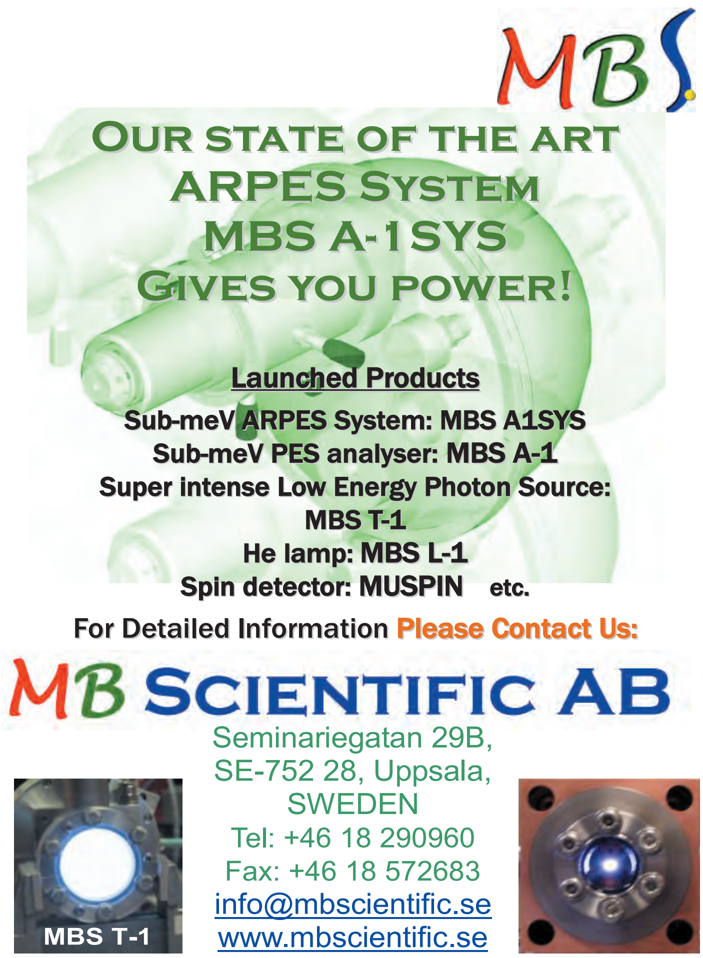
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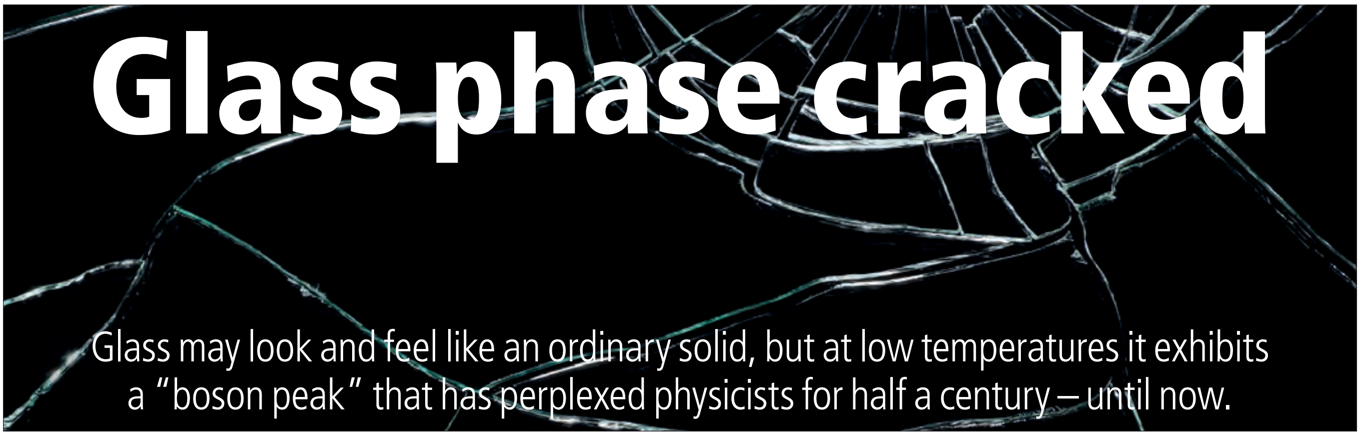


Glass phase cracked

Glass may look and feel like an ordinary solid, but at low temperatures it exhibits a "boson peak" that has perplexed physicists for half a century – until now.

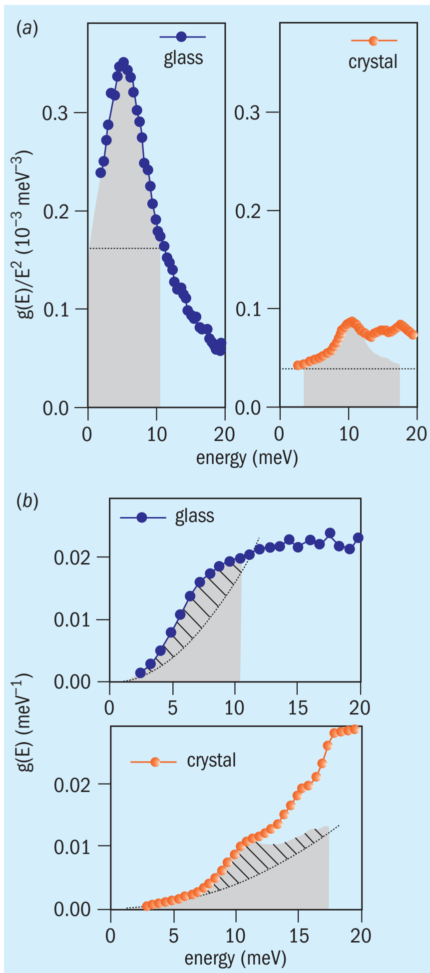
Tap a solid object such as a desk, and you will generate a sound – a pressure wave that spreads out with a certain speed. The faster you tap, the shorter the wavelength, but the speed of sound remains constant. This is the basis of the 100-year old Debye model, which allows us to calculate the degrees of freedom (or the number of vibrational states) in a system and therefore the heat capacity of any solid, just from the speed of sound and the number of atoms in the sample.

When the wavelength of sound waves becomes comparable with the period of the crystalline lattice, however, this picture starts to break down and the Debye theory predicts an accumulation of vibrational states at certain frequencies and thus an increased heat capacity. Unlike a crystalline solid, glasses are disordered and therefore are not expected to exhibit this short wavelength behaviour: the Debye model should hold.But experiments in the 1960s revealed otherwise. At temperatures of around 10 K where, oddly, crystals do not show much deviation from the Debye model, the heat capacity of glasses rises significantly above the Debye prediction. This extra heat capacity means that one needs to put extra energy into a glass to heat it to a given temperature, and suggests that a glass has additional vibrational states into which you can put that additional energy. The additional vibrational states became know as the "boson peak".

For the past 50 years, physicists have tried to understand the physical origin of the boson peak, and thus how disorder in atomic positions makes glasses so different thermodynamically from ordered crystals. But despite dozens of theoretical models and hundreds of experimental results, no unified picture emerged. "If you Google 'boson peak glass' you will have over 100,000 hits," says Alexander Chumakov, scientist on the ESRF's ID18 beamline. "Some people call it the last puzzle of solid state physics."

Unexpected result

In experiments carried out at the ESRF on beamlines ID18, ID27 and ID28, Chumakov and co-workers claim to have solved the riddle of the boson peak. The international team compared atomic motions in a glass



The Debye model predicts that the density of states, g(E), at low energy is proportional to E^2, so the reduced density of states ($g(E)/E^2$, top) should be a straight line. Glasses exhibit an excess of $g(E)/E^2$ compared to crystals, but the total number of states (the area bounded by g(E), bottom), is the same: the boson peak in the glass has no additional modes over the crystal.

with those in a corresponding crystal using nuclear inelastic scattering, a technique that determines the exact number of vibrational states. Remarkably, the number of states measured around the boson peak turned out to be exactly the same as the number of the corresponding acoustic degrees of freedom in a crystal (*Phys. Rev. Lett.* **106** 225501).

"The very concept of these extra degrees of freedom where you have to put the energy of the extra heat capacity turned out to be incorrect," says Chumakov. "The additional heat capacity is not because of additional vibrational states but because the same states are located at lower energy and, thus, are more efficiently activated at lower temperatures. The behaviour is not anomalous, it is the same as for crystals but just appears at lower temperatures."

Convincing the community?

The team's dramatic conclusion, which stemmed from pioneering investigations of glass dynamics in the mid-1990s at former inelastic X-ray scattering beamline ID16 by the ESRF's Giulio Monaco and Francesco Sette, emerged from careful comparisons between an iron-containing sodium silicate glass, $Na_2FSi_3O_{8.5}$, and a crystal of a similar composition and density. To some, that's a relatively exotic form of glass. So the ESRF-led team has recently performed the same experiment with the very material that launched the boson-peak mystery 50 years ago: plain old window glass, SiO_2. Exactly the same agreement between the number of vibrational states in glass and its corresponding crystal was observed.

The work is a big leap forward, but the book is not closed on the boson peak, according to Reiner Zorn of the Jülich Center for Neutron Science in Germany. "Although the ESRF results leave open the possibility that there is something in addition to transverse waves, there is now no necessity to assume such boson-peak specific vibrations," he says. "Such measurements have a long tradition in inelastic neutron scattering, but for that method the high pressures necessary here are currently out of reach."

The glass phase has further riddles in store, says Chumakov. "Glasses possess many other intriguing features still waiting for clarifications, for instance the so-called "fast processes", correlated diffusion, dynamic heterogeneities, and many others that will be attacked soon by ESRF researchers and users."

Matthew Chalmers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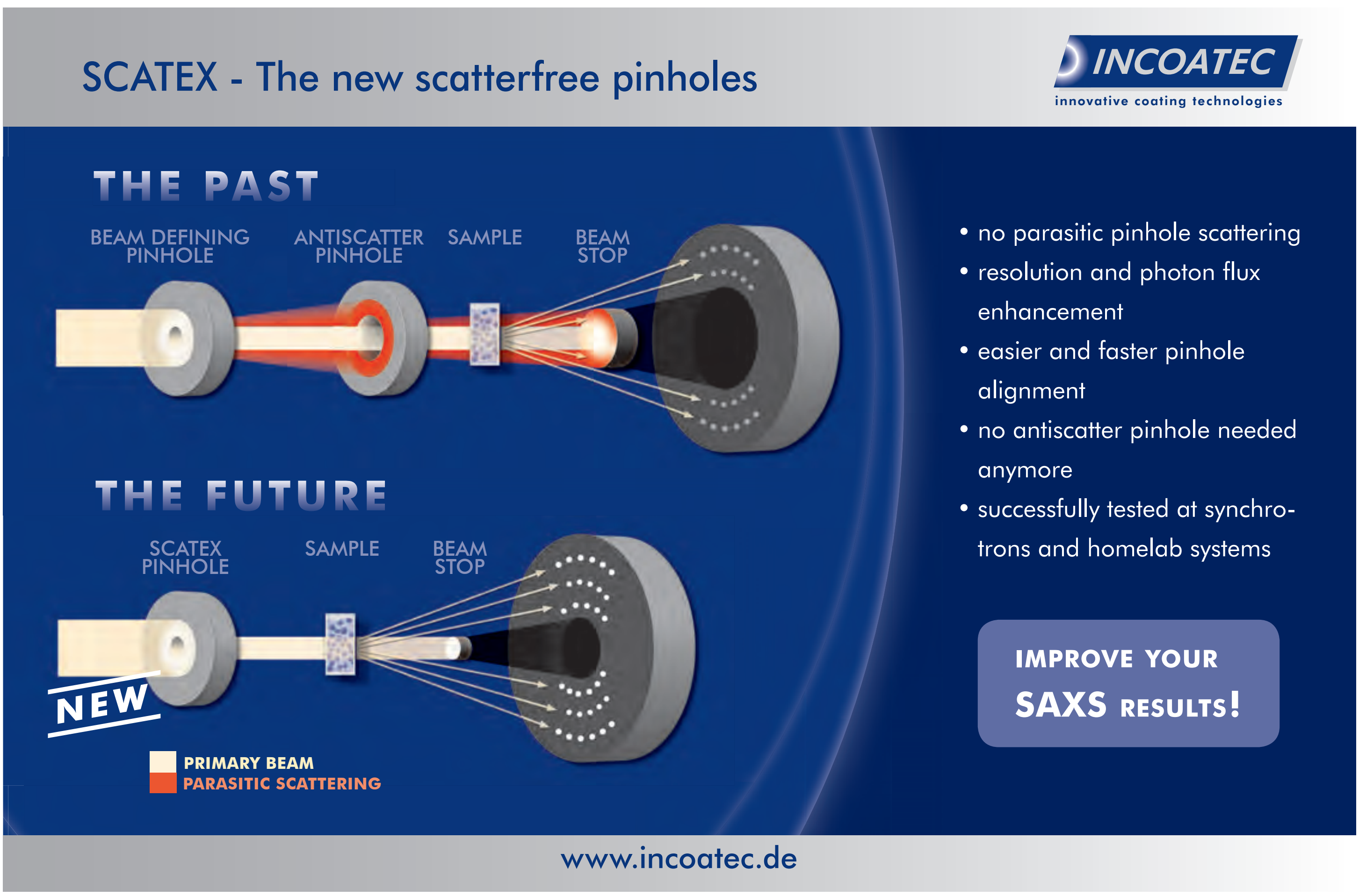
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Stellar insight

A geometric representation of quantum mechanics developed by ESRF theorist *Patrick Bruno* tames the abstract world of magnetic systems.

Niels Bohr, a leading architect of quantum mechanics, famously remarked that anyone who was not shocked by quantum theory had not understood it. Today, quantum mechanics remains as weird and counterintuitive as ever, helped only by a strong command of mathematics. Sometimes even the best mathematical minds need help to work what it means.

Head of the ESRF's theory group, Patrick Bruno, has found a way to represent complex quantum systems in a relatively simple geometric form. Based on a powerful but largely ignored concept invented by Italian physicist Ettore Majorana 80 years ago, Bruno's formulation offers a deeper insight into the behaviour of magnetic "spin" systems.

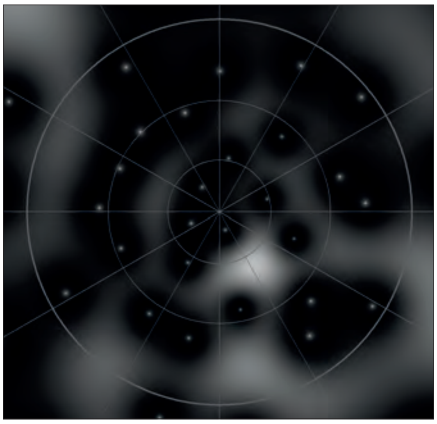
Physical picture

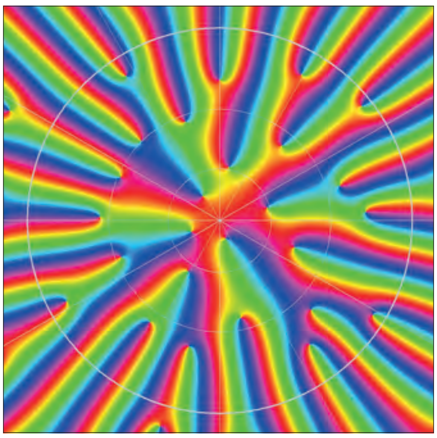
Aged 26, Majorana devised an elegant representation that described a pure quantum state of a spin-J system, where J is the spin, as a constellation of $2J$ points on a sphere, analogous to stars on the celestial sphere. The result was contained in one of just 10 papers that Majorana published in his short but influential career; six years later he would board a boat on the island of Palermo bound for Naples, and mysteriously disappear.

Spin is a measure of the intrinsic angular momentum of a quantum system. A spin ½ system such as a single electron has two levels: ± ½, commonly called "up" and "down". The standard way to represent this, using Schrödinger's wavefunction or Heisenberg's matrix formulation of quantum mechanics, is in terms of $2J+1$ complex numbers. This representation not only becomes complicated for higher spin systems, but there is no way to get a perception of what it means physically.

"You don't care about lists of complex numbers moving on the screen on your computer," explains Bruno. "In classical mechanics, motion is a point moving from one place to another in time, and the difficulty in quantum mechanics is to create that geometric picture."

Being purely geometric, Majorana's representation recovers the concept of a trajectory in quantum mechanics. The basic states of a two-level system correspond to a unique star at the "north" and "south" poles, and linear superpositions of theses states correspond to the star being located anywhere on the sphere. This is the familiar Bloch representation and is the essential ingredient of a qubit, the basic element of quantum information processing. "Manipulating qubits just means doing certain rotation operations on one point on a sphere," Bruno explains. "More realistic systems have more than two levels, and the question is: how do we represent that in a geometric manner?"





Top: Stereographic representation of the quantum state of a spin system with J=25, where the dots are Majorana stars and the hazy regions depict the density of a fictitious classical gas. Bottom: Map of the phase of the wavefunction of the same spin state, in which the stars appear as phase singularities.

The ESRF in theory

The ESRF's theory group currently comprises four staff who conduct research into theoretical physics, mainly solid-state theory and magnetism, and assist users and beamline scientists. Calculations performed last year by a PhD student in the group, for instance, helped understand high-pressure studies of the magnetic behaviour of nickel at the ID24 beamline (*Phys. Rev. Lett.* **107** 237202). The group also works alongside theorists from the Institut Laue-Langevin. "It is quite a unique environment," says Bruno. "We are not expert in all experimental areas, but my door is always open and people are welcome to expose us to new problems."

This year, Bruno found a way to express the expectation value of physical observables in a spin-J system, for instance its dipole moment and energy, in terms of the Majorana stars. He used a novel diagramatic method by which he was able to map the quantum state of any spin-J system onto the thermodynamic partition of a fictitious classical gas on the sphere (*Phys. Rev. Lett.* **108** 240402).

Having shown how to derive the observables of a spin system for a given configuration of stars, Bruno also worked out the "symplectic structure" of general spin-J systems. This structure, which in quantum mechanics is given by the geometric phase (a phase shift acquired by a system upon cyclic motion of the stars on the sphere), determines how a system evolves in response to forces, and thus determines its dynamics.

Synchrotron tests

Essentially, Bruno has found the quantum mechanical counterpart of the well known Landau–Lifshitz equation, which describes the precession of an electron in a magnetic field and is the basis for understanding magnetic systems such as computer hard disks. He is now working on a second, longer, paper in which he will set out the applications of his new formulation. "Usually one is interested in systems that are more complex, such as infinite lattices of spins coupled together by exchange interactions, so it could be a ferromagnet for instance. I will be then able to describe systems that people investigate with neutrons or X-rays."

The work will be particularly useful, he says, for making sense of experiments with nematic magnets, which the Landau–Lifshitz equation cannot solve because they contain states with zero magnetic moments. "This paper will presumably be much less cited than many other things that I have done, but it's one with which I am particularly happy."

Theorist John Hannay of the University of Bristol, UK, who has carried out similar work, told *ESRFnews* that he was delighted when he learned of Bruno's "very imaginative and neat re-interpretation" of the theory of Majorana stars. "I would not say my work, or his re-interpretation, impinges on any deep or philosophical problems of quantum mechanics, though I might hope that it indeed could possibly be useful in qubits or exotic magnets."

Matthew Chalmers

An interview with nature

Fundamental questions that you probably never thought to ask are being addressed in experiments at the ESRF.

Can light shine through walls?

It took 10,000 physicists and a €6 bn collider to discover the Higgs boson at CERN, but there are easier ways to search for some elementary particles. One is to shine X-rays through a magnetic field and onto a solid wall that has a photon detector on the other side. Classically, no light gets through. But quantum theory allows a virtual photon produced by the magnetic field to combine with a real photon in the beam and form an "axion", a weakly interacting boson invented to solve problems in particle physics and cosmology. The axion would travel through the wall unimpeded and be converted back into a real photon by interacting with a second virtual photon on the other side.

In 2010, researchers from the ESRF and the Laboratoire National des Champs Magnétiques Intenses in Toulouse searched for such photon regeneration using 50–90 keV X-rays at the ESRF's ID06 beamline. Two superconducting magnets produced a 3T field on either side of a 50 mm-think lead shutter, with a high efficiency germanium detector located on the far side (*Phys. Rev. Lett.* **105** 250405).

Alas, no signal was observed. But with the ESRF's photons being so energetic the work places a new lower limit on the axion mass: 17 MeV/c^2. The experiment was a first for synchrotrons, says team member Carsten Detlefs of the ESRF. "With X-ray experiments you can exclude higher axion masses because the axion mass is much smaller than the photon energy, which in laser or microwave experiments is pretty small."

Why does an electron gas form at interfaces?

Interfaces between transition metal oxides can exhibit electronic properties that are absent in the individual layers, a prominent example being the formation of a conducting electron gas between the insulating compounds $LaAlO_3$ and $SrTiO_3$. In an attempt to explain this unusual behaviour, X-ray absorption spectroscopy carried out at the ESRF's ID08 beamline in 2009 allowed researchers to probe the electronic properties and orbital structure of the interface (*Phys. Rev. Lett.* **102** 166804). The results showed that a structural distortion appears at the interface and in particular that the formation of a conducting 2D electron gas is related to an orbital reconstruction during which the degeneracy of titanium's 3*d* electronic states is removed.

Is the speed of light the same to all observers?

That the speed of light is a fundamental constant is the core of Einstein's special theory of relativity, ensuring that space-time is Lorentz invariant and therefore looks the same no matter which direction you travel in. But this fundamental symmetry might not hold at the most extreme subatomic scales, where uncertainty reigns and nature is thought to be governed by the laws of quantum gravity.

An experiment called GRAAL – GRenoble Anneau Accelerateur Laser – installed at the ESRF several years ago allowed physicists to search for cracks in Lorentz symmetry by studying the Compton backscattering of laser photons off electrons in the storage ring. Electrons and photons collide such that the photon is bounced back and gains energy while the electron loses energy via Compton scattering. Since the energy loss of the electron depends sensitively on the speed of light, any directional variations in the speed of light would show up in the electrons' energy loss. The team monitored the electron energy loss continually for 24 hours to see if the it changes as the Earth rotates, and the results were published in 2010 (*Phys. Rev. Lett.* **104** 241601). No variations were spotted, placing new limits on anisotropies in the propagation of light at the 10^{-14} level, as expressed in terms of coefficients in a Lorentz-violating extension of quantum electrodynamics. That's 10 times better than previous experiments and "represents a billion-fold improvement over the original test performed by Michelson and Morley in 1887", says co-author Ralf Lehnert of the National University of Mexico.

What do quantum effects look like at macroscopic scales?

The Lamb shift, observed by US physicist Willis Lamb in the late 1940s, is a small correction to the $^2S_{1/2}$ and $^2P_{1/2}$ energy levels in the hydrogen atom caused by the emission and reabsorption of 'virtual' photons from the vacuum. This causes a tiny shift in the frequency of a spontaneously emitted photon that agrees with the predictions of quantum electrodynamics to one part per million. But when an atom is one of an ensemble, the emitted photon may also be absorbed by other identical atoms – with dramatic effect. The "collective" Lamb shift is predicted to cause a strong acceleration of the collective emission called superradiance, but the effect is extremely difficult to observe in the optical regime.

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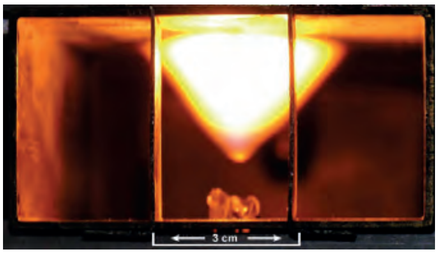
The Lamb shift has been observed en masse.

In 2010, an experiment at the ESRF's ID22N beamline led by physicists from DESY demonstrated a simple way to observe superradiance and the collective Lamb shift in the X-ray regime (*Science* **328** 1248). The team embedded ultrathin layers of ^{57}Fe (a two-level Mössbauer isotope) between two mirrors spaced a few nanometers apart and resonantly excited them with X-ray pulses. Multiple reflections of the radiation within the cavity cause the ensemble of atoms to appear optically thick, and once it was excited into a purely superradiant state, the researchers found that the ensemble decayed almost two orders of magnitude faster than a single atom – in excellent agreement with calculations.

What is ball lightning?



A stable fireball in a microwave cavity.

Ball lightning – a slow-moving orb of light seen hovering above the ground during thunderstorms – has puzzled scientists for a century. It is thought to be a plasma formed when lightning hits the ground and creates a hot-spot, ejecting a plume of silicon, silicon-oxide and silicon-carbide nanoparticles that sustains an optical glow.

To mimic these reported atmospheric events, a team from the University of Rennes, the ESRF and Tel Aviv University used a fireball generator that channels microwaves through a rod into a solid substrate made from glass or some other ceramic (*Phys. Rev. Lett.* **100** 065001). Small-angle X-ray scattering at the ESRF's ID02 beamline allowed the team to probe the structure of the fireball as it evolved, revealing it to be a dusty plasma consisting of charged nanoparticles with a mean size of 50 nm.

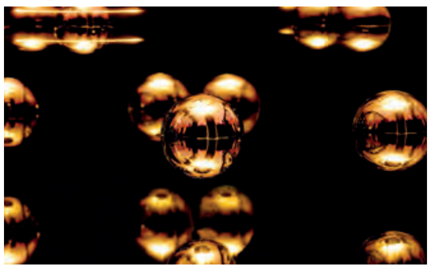
According to other physicists, however, the mystery of ball lightning is a matter of the mind. Recently, Josef Peer and Alexander Kendl of the University of Innsbruck claimed that the phenomenon is an illusion caused by the large magnetic fields created by ordinary lightning (*Physics Letters A* **374** 2932). "We conclude that a plausible interpretation of a large class of reports of luminous phenomena during thunderstorms is the result of electromagnetic pulse induced transcranial magnetic stimulation of phosphenes in the human brain."

What happens when a fluid goes supercritical?

As a substance goes beyond its critical point at high temperatures and pressures, it enters a single "supercritical fluid" phase in which there is no way to distinguish the gas and liquid states. At least, that's what the textbooks say. In 2010, using inelastic X-ray scattering and molecular dynamics simulations at the ESRF's ID28 beamine, a team lead by researchers from the universities of Rome and Florence identified two distinct dynamical regimes (liquid-like and gas-like) in dense, hot supercritical fluid argon, revealing for the first time a crossover between liquid-like and gas-like behaviour (*Nature Physics* **6** 503).

A sharp decrease in the dispersion of sound waves observed at pressures of 0.4 GPa, due to the disappearance of the structural relaxation process, marked the transition from a collective liquid-like to a single particle gas-like behaviour, claims the team. This provides a connection between dynamics and thermodynamics and contradicts the widespread belief of a homogeneous supercritical fluid phase. The crossover corresponds to the extrapolation of the so-called Widom line, which constitutes the locus of maxima of the isobaric specific heat capacity in the supercritical fluid phase. "This offers the first fundamental insight into the correspondence between subcritical and supercritical fluid behaviour," the team concludes. "These findings open up new territory for which there is at present no theoretical framework."

What is the smallest atomic displacement?



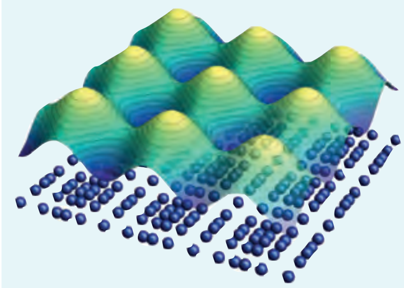
GHIANDONI AND PAOLASINI

Femtoscale atomic displacements hold the key to multiferroic behaviour.

Multiferroic materials have the unusual property that they can be both magnetically and electrically ordered. In an attempt last year to understand what drives this behaviour, a team led by the ESRF's Helen Walker showed that the electric polarisation in multiferroics is caused by the relative displacement between charges of different signs. Magnetic polarisation, by contrast, is driven by the alignment of the individual magnetic moments of the atoms in a magnet.

The team's insight came from a new technique that exploits the interference between two competing processes: charge and magnetic scattering of a polarised X-ray beam. With it they were able to measure displacements of specific atoms in a single crystal of $TbMnO_3$, which exhibits multiferroic behaviour at temperatures below 30 K, as small as 20 femtometres (about 1/100,000th of the distance between the atoms in the material). Because the displacement involves a high number of electrons, even small displacements can cause significant electrical polarization (*Science* **333** 1273). "I think that everyone involved was surprised, if not staggered, by the result that we can now image the position of atoms with such accuracy," said team member Des McMorrow of the London Centre for Nanotechnology.

Matthew Chalmers



Charge density waves distort the crystal lattice (blue) and compete with superconductivity.

What drives high-temperature superconductors?

Superconductivity, a state of zero electrical resistance exhibited by many elements at very low temperatures, was observed in 1911 in the metal mercury. Half a century later, physicists discovered the microscopic mechanism that drives this exotic and highly useful behaviour: correlations between pairs of electrons at low temperatures, as described by the Bardeen–Cooper–Schrieffer (BCS) theory. But in 1986, astonished physicists discovered superconductivity at much higher temperatures in more complex copper oxide or "cuprate" systems, which has puzzled researchers ever since.

Recently, an international team used resonant soft-X-ray scattering at the ESRF's ID08 beamline to help identify 2D charge fluctuations in the copper-oxide planes of ceramic yttrium and neodymium barium cuprates (Y, Nd)$Ba_2Cu_3O_{6+x}$. Understanding charge, spin and orbital correlations in the normal state from which superconductivity emerges is key to finding a successful theory of high-temperature superconductivity in the cuprates, which could help researchers exploit this property for more efficient engineering materials, and it is suspected that ordering phenomena are a key factor. A long-standing debate concerns whether "stripe ordering", a type of antiferromagnetism, is a generic feature of the cuprates and thus whether stripe fluctuations are essential for superconductivity. The ESRF result, taken together with data from the Swiss, Canadian and BESSY light sources, indicates that the correlation length of the charge fluctuations increases as the temperature is lowered and then reverses at the transition temperature, indicating an incipient charge-density wave instability that competes with superconductivity (*Science* **337** 821).

"We did not expect the charge density waves in the superconducting cuprates because they destroy the superconductivity," says team member Bernhard Keimer of the Max-Planck-Institute for Solid State Research in Stuttgart. "Superconductivity only just prevailed in this competition."

Spanning the generations

Managing director of the European X-ray free electron laser, **Massimo Altarelli**, surveys the landscape of next-generation light sources.

When you are young and foolish, you make some choices that influence the rest of your life. That's what Massimo Altarelli says of his decision to train as a theoretical physicist in the 1960s. "Italian physics is very much shaped by the image of Enrico Fermi, and theoretical physics had a strong reputation," he explains. "I also have an elder brother who is a theoretical particle physicist at CERN – he gave me the virus."

In January 1987 Altarelli became the ESRF's first research director. At the time, the facility's dozen or so staff were located in a single prefabricated "barrack", and Altarelli's main task was to shape the beam-line portfolio and recruit scientists. By the time he stepped down in 1993 there were 160 staff in the experiment division, including now director general, Francesco Sette. Altarelli had little experience of management though, he recalls. "I just applied common sense, and people seemed to like it."

Altarelli also established the ESRF's theory group, which he led until 1999. But after returning to Italy as director of the Elettra light source in Trieste, his attention turned to next-generation light sources. In 2006 he took up a position at DESY in Hamburg, where the free-electron laser FLASH had just turned on, as project leader of the European X-ray free electron laser (XFEL).

EUROPEAN XFEL

Massimo Altarelli in brief

Born
Rome, 1948.

Career
- **1969–1971** fellowship, Italian National Research Council, Italy
- **1971–1973** postdoc, University of Rochester, US
- **1974–1979** assistant professor, University of Illinois, US
- **1980–1987** scientist, MPI for Solid State Research, Germany
- **1987–1993** ESRF research director, Grenoble, France
- **1994–1999** head of the Theory Group, ESRF
- **1999–2004** director, Elettra Light Source, Trieste, Italy
- **1999–2006** staff member, ICTP, Trieste
- **2006–2009** leading scientist, DESY, Hamburg, Germany
- **2009-present** managing director, European XFEL GmbH, Hamburg, Germany

"It takes a lot of time, effort and wheeling and dealing."

Growing family

XFELs accelerate bunches of electrons to high energies before channelling them through undulators to produce short and intense bursts of self-amplified spontaneous synchrotron radiation. FLASH was the world's first soft X-ray laser, but the European XFEL currently being built next door will take the technology into the hard X-ray regime. Recently, the European XFEL's tunnels were completed and the equipment to fill them is currently being procured and installed. When it turns on in 2015, the facility will join the LCLS in Stanford, US, and SACLA in Japan.

"The XFEL family is growing fast," says Altarelli, with two being built in Switzerland and Korea, and plans for one in China. "People often call these fourth-generation light sources, but they work on a completely different principle – it's a jump in the evolution of the species." That said, he admits that the overwhelming know-how for X-ray lasers comes from third-generation synchrotrons.

The peak brilliance of XFELs is at least eight orders of magnitude higher than that of third-generation sources, which allows crystallography on samples well below a micron in size. The extraordinary short pulse durations of XFELs, of the order 10 fs, also allow extreme time-resolved experiments for monitoring chemical reactions and phase transformations in real time.

But as more XFELs switch on in the next few years, third-generation facilities – notably the ESRF – are gearing up to turn their equipment into "ultimate storage rings" that will boost their brilliance. Will this present competition for XFELs? "Even ultimate storage rings will not have the peak brilliance or timescales that we have, but there is a machine that exists only on paper that could compete with both XFELs and storage rings," says Altarelli.

Seeding the future

That machine is called an energy recovery linac, which recycles the electrons' energy rather than using it only once in single-pass mode. This reduces the energy bill, explains Altarelli, and allows undulators to be inserted into the bends of the accelerator, but construction costs are still prohibitively high. "There will be a move towards more compact and efficient XFELs," he says. Seeding, a mechanism whereby the lasing process is not triggered by random fluctuations but by a monochromatic "seed" pulse, is eventually going to take over, thinks Altarelli, because it produces higher quality pulses. "Another thing we will see in the next decade is continuous-wavelength operation."

The European XFEL will use superconducting cavities, which suffer fewer losses than those used at LCLS and SACLA, and therefore enables higher pulse repetition rates. Indeed, although the design of the European XFEL was very conservative, the Hamburg team knows that it can now look forward to pulses with wavelengths as short as 0.04 nm – three times less than at the LCLS.

When the LCLS started up, says Altarelli, over half its users were from Europe. But despite the scientific potential of the European XFEL, in which Germany and Russia hold a 60% and 25% stake, respectively, Altarelli thinks that some European countries are underestimating its importance. "It takes a lot of time, effort and wheeling and dealing to reach political consensus," he says. "But in the end it will be worth it to have in Europe the fastest, most powerful light source ever constructed."

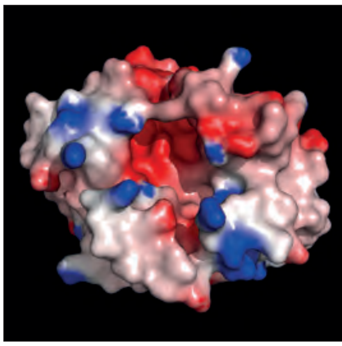
Matthew Chalmers

Flu structure heads to market

Savira pharmaceuticals has teamed up with Roche to develop new influenza drugs following groundbreaking structural studies performed at the ESRF.

Each year hundreds of thousands of people die from seasonal outbreaks of influenza, and every so often a global flu pandemic takes the lives of many more. There is no vaccine that is 100% effective, nor a cure. But antiviral drugs can help reduce symptoms and minimize the spread of flu.

The ESRF played a vital role in elucidating the structure of targets in the virus replication machinery, namely the "cap-snatching" process. Here, a viral enzyme called polymerase cleaves off a small chemical structure called a cap from the host cell's protein coding RNA (mRNA), causing its protein-synthesis machinery to preferentially make viral proteins.

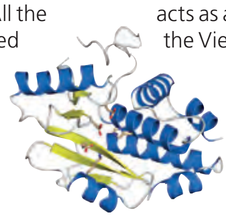


3D image of the "PA" protein domain where the cleaving of human genetic code by the flu virus takes place. The hollow canyon in the centre captures the long mRNA strand and the metal complexes at the top edges of the canyon cut off the cap. Colours denote the electrostatic surface charge.

EMBL-UVHCI

In 2007 and 2008, experiments carried out by Stephen Cusack, head of the European Molecular Biology Laboratory (EMBL) in Grenoble, and colleagues at the joint EMBL-Grenoble University-CNRS Unit for virus host cell interactions (UVHCI), revealed the two sites in the polymerase structure where cap-snatching takes place (*Nature* **458** 914; *Nature Structural and Molecular Biology* **15** 500). This opened the door to structure based anti-influenza drug design, since by inhibiting the cleaving of host RNA the virus can no longer multiply. Since all influenza strains employ the cap-snatching mechanism, such inhibitors could potentially tackle a wide range of flu viruses including novel pandemic strains.

"We knew about this process for 30 years, and I've been working on it for 15 years, but to make progress new technologies had to be invented to identify the domains responsible for cap-snatching," says Cusack, who trained as a theoretical solid-state physicist before turning to biology. All the structures were solved at the ESRF and there have been several follow-up studies since then. Now, says Cusack, his team wants to study the complete polymerase ensemble, rather than small parts of it, to understand how the whole viral replication machinery works. "It is a real challenge to crystallize this very dynamic particle."



Key domain of flu virus polymerase with active site shown in red. Credit: S Cusack/EMBL.

Spinning out

In 2009, after EMBL researchers had submitted patent applications covering the use of the two structures for drug design, Cusack co-founded Savira pharmaceuticals to develop antiviral compounds. Today he acts as an unpaid consultant to the Vienna-based firm, which employs 10 people. "I just want our research to be put to use to improve public health," he says. "This is best achieved by both academics and industry working together as it's really expensive and requires a lot of expertise to turn an inhibitor into a drug."

Earlier this year Savira signed an agreement with Roche, which manufactures the antiviral influenza drug Tamiflu, to provide an exclusive license on its cap-snatching inhibitor program. In return, Savira will receive funds that could total €240 m in addition to upfront payments, research and development support and eventual royalties.

"Stephen and his team's work at the ESRF laid the basis of Savira's rational drug design programs," says Savira CEO Oliver Szolar, who expects that it will take at least six to eight years before one of Savira's flu polymerase inhibitors reaches market, following extensive toxicology studies and clinical trials. "The ESRF is still of great interest to us in this early stage," he says. "Future structural information will still impact our development, but soon the program will move into the clinical phase."

Matthew Chalmers

Movers and shakers

Directors' corner

Bauke Dijkstra is the ESRF's new director of research for life sciences, beginning his five-year term in September. Since 1993 Dijkstra has been a professor of biophysical chemistry at the University of Groningen in the Netherlands, with research interests in enzyme catalytic mechanisms, protein engineering and biotechnology. He first came to the ESRF as a user in the mid-1990s and members of his group have been frequent visitors. Dijkstra, who is an associate editor of the *Journal of Structural Biology*, told *ESRFnews* that it's an exciting time to arrive at the ESRF. "People are very supportive and it is a very active group with many ideas."

Luis Sánchez-Ortiz has returned to the ESRF as director of administration. He first came to the ESRF in 1995 as internal auditor, leaving six years later for the Spanish Foundation for Science and Technology. From 2007, Sánchez-Ortiz worked in the private sector.

Synchrotron Knight

Christian Vettier has been made Chevalier de la Légion d'Honneur – Knight of the National Order of the Legion of Honour – for his contributions to the European Spallation Source project in Lund, Sweden. Vettier joined the ESRF in 1990 and established the magnetic scattering beamline ID20, later becoming head of the magnetic scattering group. He remains a consultant to the ESRF. The prestigious medal was awarded at a ceremony in Stockholm in September.

UK fact-finding visit

On 5 September, five members of the UK's large facilities steering group (LFSG), which oversees and determines the level of UK funding for facilities such as the ESRF and ILL, visited the ESRF. "Overall, LFSG felt that the visit was a very positive experience," says Jennifer Scratcher of the UK's Science and Technology Facilities Council.

"We were impressed with the dynamic nature of the facility and felt there was a real 'buzz' when touring around and talking to the instrument scientists."

Crocs up close: These stunning images, obtained using propagation phase contrast imaging at the ESRF's ID19 beamline, show a 31-day-old embryo of a Nile crocodile (*Crocodylus niloticus*). The left panel shows the external morphology of the creature, which was obtained from the Crocodile Farm in Pierrelatte, France, while a semi-transparent view (right) shows the skeletal mineralisation (the embryo measures 1.4 cm across). Crocodiles belong to the group of ancient reptiles, which evolved into an astonishing variety of different forms – the most interesting morphological transition being the emergence of feathers. "To understand the embryonic life of dinosaurs, we need to understand that of their closest living relatives first," says Martin Kundrát of Uppsala University in Sweden, who led the research in conjunction with the ESRF's Paul Tafforeau. "This quantitative knowledge is essential for understanding ancient embryonic development and its bearing on the evolution of bird-like features in dinosaurs."

In the corridors

Astronomical anniversary

The Crab nebula at X-ray (blue) and optical (red) wavelengths.

X-ray astronomy was born 50 years ago this year, with the discovery of the first extra-solar X-ray source: "Sorpius X-1". This compact object lies about 9000 light-years from Earth and, apart from the Sun, is the strongest source of X-rays in the sky. Its discovery, which won Italian astrophysicist Riccardo Giacconi a share of the 2002 Nobel Prize for Physics, opened a new window on the universe that today is being probed by dedicated X-ray observatories including the XMM-Newton and Chandra space missions.

Employers prefer men to women

Researchers at Yale University have published a study showing that scientists rate male job applicants more highly than females ones (*PNAS* **109** 16474). The team asked 127 biology, chemistry, and physics professors in the US to evaluate the job application of a fictitious undergraduate science student who had ostensibly applied for a laboratory manager position. Half received applications attributed to a student called "Jennifer" while the others received identical materials attributed to an applicant called "John". Both male and female faculty members judged the female student to be "less competent and less worthy" of being hired than the identical male student, and also offered her a smaller starting salary. The findings, concludes the team, "raise concerns about the extent to which negative pre-doctoral experiences may shape women's subsequent decisions about persistence and career specialisation".

Driven by X-rays

Swedish car manufacturer Volvo has unveiled an app that turns iPhones and iPads into handheld "X-ray scanners", allowing users to see beneath the skin of its latest models. The gizmo, developed by digital agency La Comunidad in Miami, uses augmented-reality technology that allows devices to read markers placed around the car.

Celebrating crystallography

The United Nations has declared 2014 International Year of Crystallography. The decision was announced on 4 July by the International Union of Crystallography (IUCr) to mark the centenaries of the discovery of X-ray diffraction and the formulation of Bragg's Law. The ESRF will join the IUCr in planning events to stimulate and ignite interest in crystallography amongst students, scientists and the general public.

Origins of art and archeology

The 5th Synchrotron Radiation in Art and Archaeology (SR2A) symposium held in New York in June this year (*ESRFnews* July 2012, p30) was organised by the Metropolitan Museum of Art of New York, the Conservation Center at the Institute of Fine Arts of New York University, the Winterthur Museum, Cornell University and Brookhaven National Laboratory. The inaugural SR2A event in 2005 was jointly organised by the CNRS–Grenoble and the ESRF.