A LIGHT FOR SCIENCE

ESRF news

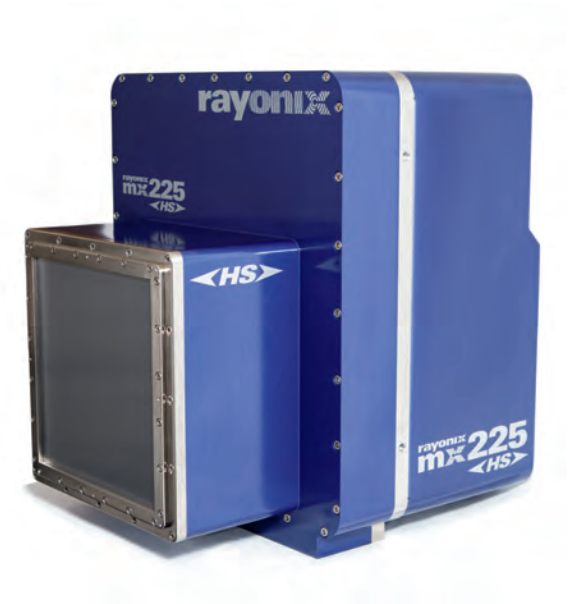
Number 67 July 2014

ESRF Upgrade Programme

The next phase

New chemistry boosts batteries

Tracking nanoparticles in the food chain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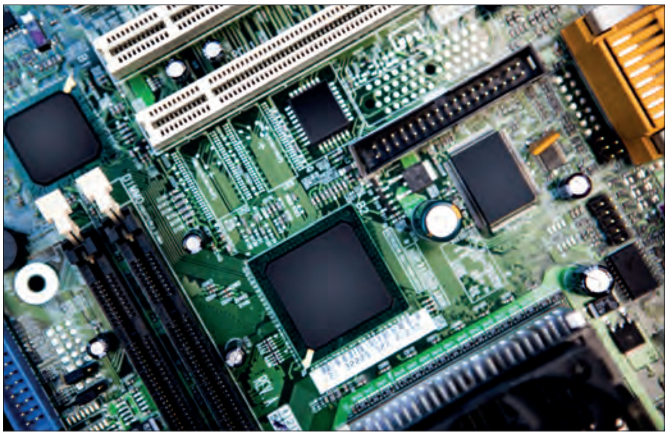

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On the cover:
View of the ESRF showing
the new buildings of ESRF
UP PI (credit: G Admans/ESRF).

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Onwards and upwards

In 2009, following 15 years of successful user operation, the ESRF launched an ambitious Upgrade Programme to help address the major scientific challenges of the 21st century and maintain the ESRF's leading role in synchrotron X-ray science. The first project phase, ESRF Upgrade Phase 1 (ESRF UP PI), has been on the European Strategy Forum on Research Infrastructures (ESFRI) roadmap since its first publication in 2006 and is currently on schedule for full implementation by the end of 2015.

ESRF UP PI is centred on the construction of new X-ray instruments and beamlines. Of 30 public beamlines and end stations spanning all user science areas, 19 are undergoing complete reconstruction or major refurbishment during the period 2009–2015. Nine new beamlines have entered user operation and two have been completely refurbished, with the remaining eight due to be finished by the end of next year.

This major upgrade has necessitated an 8000 m^2 extension of the experimental hall, meeting critical temperature and mechanical stability specifications and equipped with beamlines featuring new optics and nano-mechanics, state-of-the-art detectors, and improved computing and laboratory infrastructure. All building works are now complete, including new and improved joint premises with other institutes on the EPN campus, a visitor centre, a new site entrance and a walkway linking the ESRF and the Science Building.

A crucial strand of UP PI has been the further development of the ESRF's accelerator complex in order to improve its brightness, reliability and stability. Considered as a whole, UP PI on average allows ESRF beamlines to perform 5000 times better than before thanks to: a factor five increase in brilliance; a beam on the sample with an area smaller by a factor of around 100; and 10-times-faster detectors. A new era for X-ray science is emerging whereby users can understand and visualise the hierarchical static and dynamic organisation of complex matter from the macroscopic scale down to the nanoscale.

> **"A new era for X-ray science is emerging"**

Next step

In order to reap the full benefits of these new capabilities, the ESRF Council formed an expert working group in 2011 to study the strategic mission of the ESRF for the forthcoming 20 years. Its report concluded that, in line with the "Purple Book" objectives, the ESRF should pursue a storage-ring upgrade in the existing tunnel capable of increasing significantly the X-ray brightness and transverse coherence. Recently, the ESRF submitted a technical design study for such a machine and the science it would enable, called the "Orange Book", a summary of which is the focus of this issue of *ESRFnews* (pp14–22).

The ESRF has become a reference and inspiration for other world-class synchrotron, XFEL, extreme-light and neutron-source facilities. ESRF UP aims to provide its users with new instruments and beamlines that couple established scattering, diffraction and spectroscopy measurements to real-space microscopy and 3D imaging capabilities at the nanometre scale. This will bridge the gap between today's X-ray analytical capabilities and electron microscopy and reveal real-time dynamics down to timescales of 100 ps. With ESRF UP PI nearing completion, ESRF UP PII would set the scene in X-ray science for 2020 and beyond.

Harald Reichert
ESRF research director

Record number of new proposals

Despite inevitable disruptions to user operation caused by Phase I of the ESRF Upgrade Programme, interest from international scientists remains higher than ever. This year's March–April proposal round saw an all-time record of 1195 new proposals submitted – 100 more than the previous record set in 2008 when the full complement of ESRF beamlines was available and work on the upgrade had yet to start.

The record numbers are likely due to the enthusiasm of scientists to use the upgraded beamlines of ESRF UP PI, combined with the shutdown of PETRA-III in Germany for upgrades.

The top requested ESRF beamline was BM23 with 81 proposals, followed closely by ID13, ID10, ID12 and ID19. The new upgrade beamline complex ID16-NINA attracted more than 60 proposals despite only entering official user operation in April (branch B) and June (branch A). There were also more than 50 proposals for the new X-ray powder diffraction beamline ID22.

CRISP weighs up its future

The third annual meeting of CRISP – the "cluster of research infrastructures for synergies in physics" – took place from 2–4 June at the ESRF and ILL.

CRISP is a three-year project partly funded by the European Commission. It aims to promote joint R&D in particle accelerators, large-scale physics instruments and experiments, detectors and data-acquisition technologies and IT and data management systems. Launched in October 2011, CRISP brings together 11 large facilities listed on the roadmap of the European Strategy Forum on Research Infrastructures (ESFRI).

Successes of the project so far include the development of diagnostics tools for superconducting accelerator cavities, common methods and protocols for the study of macromolecular systems using neutrons and X-rays, and the deployment of the Umbrella user authentication system. "Reviewing the project, CRISP has been essential to bring different communities together," says Michael Krisch of the ESRF, who is co-ordinator of the project.


Around 100 participants discussed the successes and future of the CRISP project at the ESRF-ILL meeting.

Keynote speaker and ESFRI chair John Womersley, who is chief executive of the UK's Science and Technology Facilities Council, said: "The CRISP project is an excellent example of how major research infrastructure projects in related areas can help to share both technical capabilities and policy experience. The European Commission also understands the value and will continue to support this kind of clustering activity in Horizon 2020."

Other keynote speakers at the two-day event were Alex Müller of the CNRS, who discussed the SPIRAL2 and FAIR facilities, and Lyn Evans of CERN who spoke about the design and construction of the Large Hadron Collider.

Users' corner

At the last proposal submission deadline on 1 March, a record 1195 new proposals were received, requesting a total of nearly 17,000 beamtime shifts (see article above). The next deadline for submission of standard proposals is 1 September for beamtime during the period March–July 2015.

Proposers must use the most recent Experiment Methods template available on the User Guide web pages and ensure that Experiment Reports are submitted for all relevant previous proposals. Proposers are also invited to check the status of open ESRF beamlines for the 1 September deadline at www.esrf.fr/UsersAndScience/UserGuide/Applying/beamline-status.

News from the beamlines

- Since April, two new laboratories attached to the surface-diffraction beamline **ID03** have become operational: the Electrochemistry Laboratory located in the new LOB building (LOB-023), which is open to ESRF users and staff, and the Catalysis Laboratory also located in the new LOB building (LOB-021), which is available to ID03 users and staff.
- The high-energy beamline **ID15** will run in user mode until December, when it will be closed for approximately one year for refurbishment. The canted-beamline project will see the reconstruction of three independent experimental hutches: EH1 (the high-pressure station from **ID09A**, with refurbished optics and hutch); EH2 (materials engineering, with an energy range greater than 50 keV and a new compact wiggler); and EH3 (materials chemistry applications, with an energy range of 20–100 keV and refurbished beamline optics including a new Laue-Laue monochromator, multilayer monochromator and transfocators).
- The newly upgraded high-resolution powder diffraction beamline **ID22** has re-entered user service, offering users its first official public and proprietary research in May 2014.
- **MASSIF-1 (ID30A-1)**: the first of the three high-throughput sample evaluation and data collection end-stations for structural biology at ID30 has been available for expert use since June 2014 and will open for scheduled experiments from July 2014. Potential users of MASSIF-1 have also been invited to participate in a pilot study involving completely automatic sample evaluation and/or data collection. MASSIF-1 delivers a flux of around 10^{13} photons/sec at an energy of 12.8 keV in a beam size of $100 \times 100\ \mu m^2$ at the sample position. It offers a high-capacity dewar capable of hosting 240 standard sample holders, a sample-changing robot based on a six-axis Stäubli robot and a Pilatus3 2M detector.
- Construction of the fixed-energy (12.7keV) microfocus beamline **MASSIF-3 (ID30A-3)** is nearing completion, offering the same sample-changer as MASSIF-1 and measuring diffraction data using a single-photon Eiger 4M detector with a maximum readout rate of 750 Hz. MASSIF-3 will deliver 10^{13} photons/sec in a $10 \times 10\ \mu m^2$ beam at the sample position, and will be ideal for small samples and for performing ultra-fast data collection at room temperature. Commissioning of the end-station is due to begin, and first users are expected in December 2014.
- The INS instrument on the **BM32** beamline, which is dedicated to *in situ* studies of surfaces/interfaces and nanoparticles, will be closed for upgrade from November 2014 until July 2015. A new diffractometer and a more versatile UHV/MBE/CVD growth chamber will then be available, along with enhanced coupled GIXD/SXRD/GISAXS capabilities and faster motions.

PASCAL GOETGHELUCK

The rare *Wellnhoferia grandis archaeopteryx* is the largest fossil specimen of its kind.

Fossil flight seen in new light

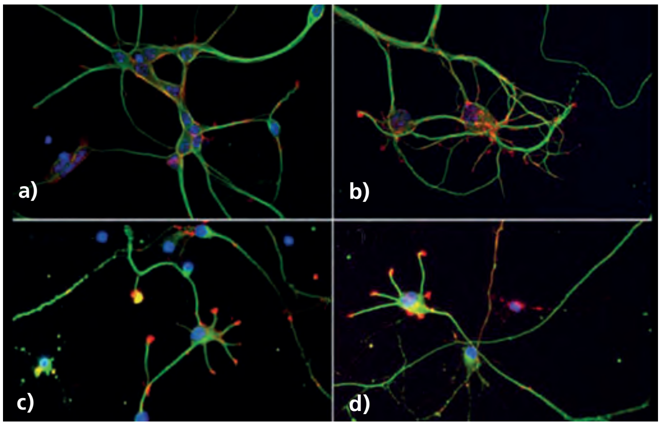
It had the teeth and claws of a dinosaur, but the feathered wings of a bird. This puzzling combination of features makes *archaeopteryx* – which lived some 150 million years ago in what is now southern Germany – a crucial species for understanding our evolutionary past.

Recent studies carried out at the ESRF's BM05 beamline reveal previously obscured features of the *archaeopteryx*, which will help scientists address the mystery of whether or not it could fly. Although its wings imply *archaeopteryx* could become airborne, the creature's body weight and certain features of its skeleton appear to contradict this hypothesis.

With only 12 known *archaeopteryx* skeletons, destructive research techniques are not applicable. Even the most powerful non-destructive imaging techniques, such as X-ray tomography, cannot be applied to *archaeopteryx* because the rock slabs in which they are embedded are often too large to be rotated in conventional scans. The new micro-beam X-ray scattering technique, which is based on the same principle as pinhole cameras, has allowed a complete 3D observation of the creature for the first time.

Developed by Anne Bonnin, now at the Paul Scherrer Institut in Switzerland, and Paul Tafforeau at the ESRF in conjunction with Martin Röper of the Bürgermeister-Müller-Museum in Germany, Dennis Voeten and Vincent Beyrand from the ESRF and Palacký University in the Czech Republic, the technique will help researchers image small features in other large and flat fossils.

Manganese maps keep MRI safe



Immuno-fluorescence labelling of mouse hippocampal neurons reveals a reduction in neuritic length as Mn^{2+} concentrations are increased from 0nM (a) to 20mM (b), 50mM (c) and 100mM (d).

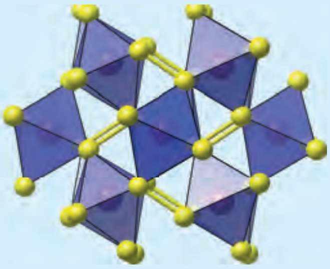
A Grenoble-based team has used the ESRF to map the spatial distribution of manganese in the brain, helping researchers assess the safety of manganese-enhanced magnetic resonance imaging (MEMRI). Manganese is an increasingly important contrast agent for MRI, which is used daily across the world to image internal body structures. The unique ability of Mn^{2+} ions – which are also essential for brain function – to trace neuronal connections and brain cyto-architecture makes MEMRI particularly effective for studying neurodegenerative diseases. But at high doses manganese is known to be toxic to the central nervous system.

To investigate these effects, Alexia Daoust of the Grenoble Institute for Neurosciences and colleagues used X-ray fluorescence microscopy at the ESRF's ID21 and ID22NI beamlines to study the presence of Mn^{2+} ions in mouse hippocampal neurons. The team submitted the cells to two doses of Mn^{2+} – a moderate dose similar to that used in brain studies and a severe dose known to be toxic – and measured the distribution of manganese and other elements (*Hippocampus* **24** 598). "This is to our knowledge the first study to provide spatially resolved information on primary hippocampal neuron manganese content," explains Emmanuel Barbier of Joseph Fourier University in Grenoble.

Results showed the presence of manganese in intracellular regions, highlighting its role in homeostasis and detoxification. At severe doses the team observed diffuse manganese distribution throughout the cell, indicating that the ability of some intracellular compartments of hippocampal neurons to store manganese is overwhelmed. The data also reveal that manganese has a negative impact on calcium and iron levels, suggesting that clinicians should use the lowest possible manganese concentration. Additional fluorescence experiments showed that manganese shortens cell extensions and decreases mitochondria velocity, suggesting that manganese may impair cell function (see figure above).

"Our approach opens new possibilities to analyse the relationship between MEMRI images and subcellular manganese content" says Barbier. "Our quantitative data also highlight the very good sensitivity of MEMRI given the use of low dose of manganese for MEMRI protocols."

Extreme collapse surprises team



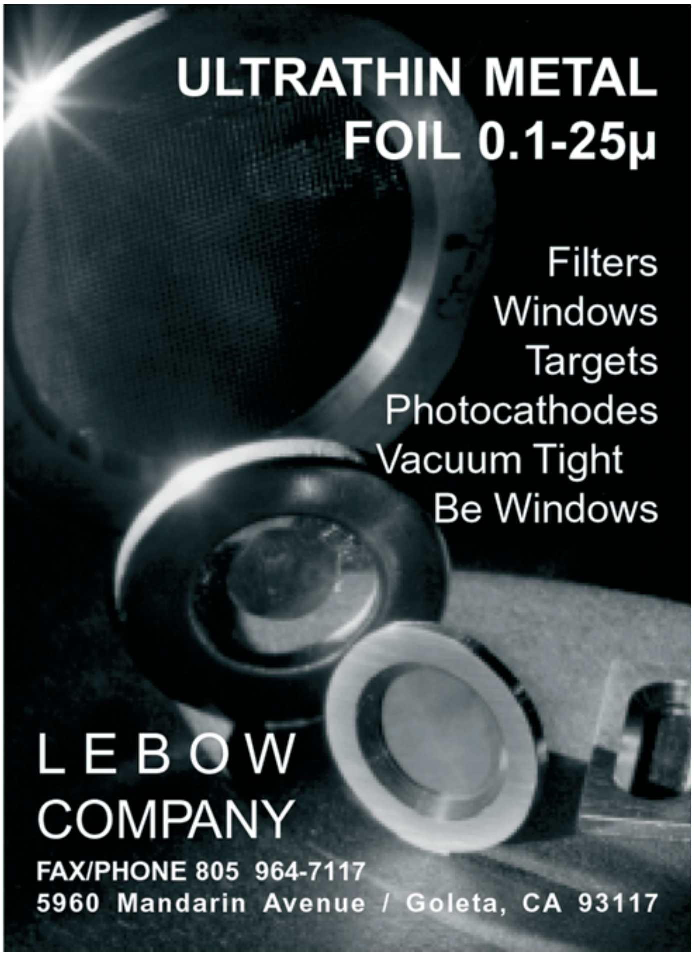
At 20 GPa, the cubic structure of MnS_2 switches to a more dense and less crystalline state.

The pyrite-like mineral hauerite undergoes a dramatic collapse at high pressure that causes its volume to shrink by 22%, an international study at the ESRF has shown. The striking effect, which dwarfs reversible structural transitions seen in any other material, points to new magnetic processes that help explain the stability of natural minerals. "When we first saw this result we were totally baffled, frankly," says lead author Simon Kimber of the ESRF.

Dramatic volume collapses under pressure are fundamental to geochemistry and are of increasing importance to hydrogen storage and high-temperature superconductivity. Most materials exhibit a smooth reduction in interatomic distances as pressure rises, but when hauerite (MnS_2) was subjected to pressures above 11.85 GPa in a diamond anvil cell at the ESRF's ID09A and ID27 beamlines its ordered crystal structure was found to almost entirely break down (*PNAS* **111** 5106).

Such collapses are usually driven by a reduction of the magnetic moment associated with individual metal atoms – so-called spin-state transitions. X-ray diffraction revealed, however, that the collapse of hauerite is driven by a different magnetic mechanism whereby Mn^{2+} cations spontaneously pair up, leading to a non-magnetic arrangement of chemical bonds. "Advances in density functional theory meant that we could actually predict changes before the experiment had even been performed," says team member Harald Jeschke of Goethe-Universität in Frankfurt.

The scale of the collapse was unexpected, though. "We have discovered a completely different way of looking at how materials shrink, and it is highly likely that other minerals will show similar behaviour," says Kimber.



Nano-probes target plant toxicity

Experiments at the ESRF are revealing the uptake mechanisms and chemical transformations of nanoparticles in living organisms, which is vital for assessing food quality and safety.

Roughly 2000 products currently available on the market contain nanomaterials, and this number is increasing. Nanomaterials display different physical and chemical properties compared to the same materials in bulk form, and the industrial applications of nanomaterials range from electronics and optics to medicine and foods. For example, Ag and TiO_2 nanoparticles (NPs) are used in outdoor paints for their antibacterial and photocatalytical properties, while Fe_3O_4 NPs have potential applications in removing heavy metals from contaminated water.

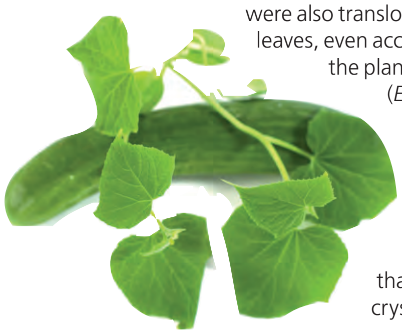
The wide use of nanomaterials raises concerns about the potential hazards of nanotechnology. Assessing the toxicological effects of NPs on living organisms is a rapidly emerging field, but knowledge about the uptake mechanisms and chemical transformations of NPs in living organisms is scarce. Since plants are a potential point of entry of NPs into the food chain, it is important that we understand such processes in order to assess food quality and safety.

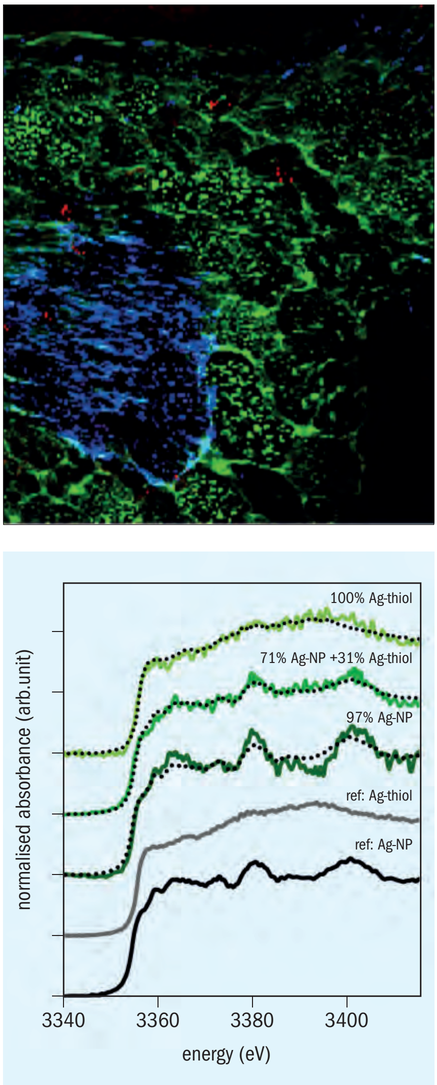
Sub-micrometre synchrotron X-ray beams offer high penetration depths and detection limits as low as femtograms per μm^2. This provides complementary information to transmission electron microscopy but without requiring ultra-thin sectioning of plant tissues. Uniquely, synchrotron X-rays can scan the absorption edge of an element with sufficient energy resolution to reveal its chemical nature. The ESRF's micro-probe beamlines ID21 and ID22 (since moved to ID16) have been deeply involved in the study of the fate and transport of toxic metals, both by external users and a strong in-house research programme.

Root of the problem

The main route of entry of NPs in plant tissues is absorption via roots. In 2012, studies of cucumber crops at ID21 using micro-X-ray fluorescence (µXRF) and micro-X-ray absorption near edge structure (µXANES) showed that TiO_2 NPs are able to reach the vascular system of cucumber roots and were also translocated to the leaves, even accumulating in the plant trichomes (*Environ. Sci. Technol.* **46** 7637). Moreover, µXANES analysis showed that certain crystalline phases of TiO_2 NPs were preferentially transported to the part of the plant that is above ground, while further experiments confirmed the presence of TiO_2 in the edible plant fruits (*Environ. Sci. Technol.* **47** 11592). Similar results showing the presence of NPs in plant roots were found in wheat and rapeseed crops (*Toxicol. Environ. Health* **75** 722 and *Sci. Total Environ.* **431** 197).

However, the behaviour of NPs also depends significantly on plant species and on the chemistry, size, shape and physicochemical properties of the NPs. For example, experiments performed last year showed that CeO_2 NPs are less mobile in rice plants (*Environ. Sci. Technol.* **47** 14110) but have higher mobility in soil-grown soybean plants. In this particular study reduced nitrogen fixation was observed and CeO_2 was found to be present in all tissues, while µXRF and µXANES studies of soybean grains revealed accumulation in the epidermal layers and no significant chemical modification of the NPs (*ACS Nano* **7** 1415).





J. HAZARD. MAT. 264 98

Top: XRF map of a lettuce leaf cross section showing Ag (red), Cl (green) and P (blue). Bottom: XANES spectra showing characteristic features of Ag NPs, revealing that they form complexes such as thiol-containing molecules.

An alternative route by which NPs can enter the food chain is foliar contamination from NP-based pesticides or after deposition of atmospheric particles. To investigate this pathway, as part of a European project called NanoHouse, we recently exposed lettuce leaves to Ag or TiO_2 NPs and used µXRF under cryogenic conditions to investigate their internalisation and distribution. Even after thorough washing of the leaves both types of nanoparticles were detected throughout plant tissue in the form of small agglomerates measuring a few microns across, demonstrating their ability to cross the leaf epidermis (*J. Hazard. Mat.* **273** 17). The TiO_2 NPs were not altered upon exposure, but µXANES revealed that Ag NPs formed new complexes with organic ligands such as thiol-containing molecules (see figure). This suggests a triggering mechanism for detoxification, although additional experiments did not highlight any acute toxicity symptoms.

3D nanoanalysis

Future experiments in this rapidly growing field will investigate the more complex interactions and movements of NPs in the food chain, for example by growing crops in agricultural soil containing NP-contaminated sewage sludge and by studying the fate of NPs on insects that feed on leaves from exposed plants. These more realistic exposure scenarios demand rapid scanning methods that can cope with larger areas and multiple samples, plus the ability to detect even lower NP concentrations.

The new nano-beamlines at ID16 that have recently come online as part of the ESRF Upgrade Programme will enable a higher spatial resolution (below 100 nm) for 2D mapping and spectroscopy, and move us towards 3D nano-analysis. The complementarity of sub-micron resolution beamlines and the existing nano-probes will allow a more detailed characterisation of NP interactions in biological systems.

Hiram Castillo-Michel, ESRF X-ray imaging group

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Fast cycling boosts lithium batteries

Microbeam X-ray diffraction reveals new chemistry in lithium-ion electrodes that could help increase the energy density of batteries.

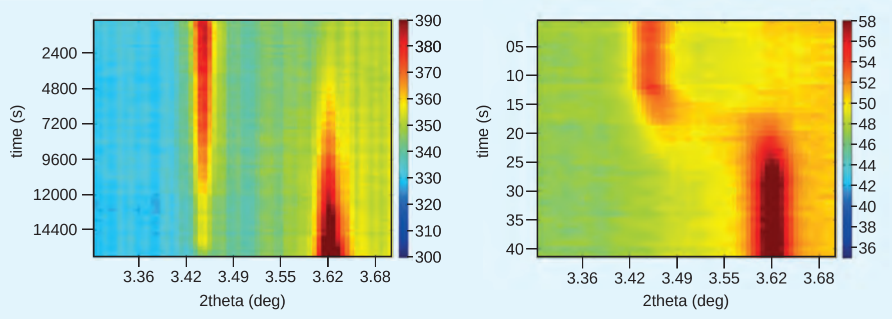
The mobile technology that has transformed our lives is often attributed to ever smaller and more powerful integrated circuits. But without high energy-density lithium-ion batteries that can be recharged multiple times, the personal electronics revolution could never have got off the ground.

Lithium, which is the third lightest element, is very small and has a tendency to give away its outer electron. This means that large numbers of lithium ions can be stored at high potentials in electrode materials such as $LiFePO_4$, making lithium-ion batteries at least three times more powerful than traditional nickel-cadmium and nickel metal hydride varieties. Because the insertion of lithium ions causes relatively small structural changes in the electrodes, the reversibility and therefore recharging rate is also much better.

Since entering commercial operation in 1991, improvements in lithium-ion batteries have been relatively slow, especially compared to the rise in computing speeds. Now a recent study at the ESRF carried out by Marnix Wagemaker and co-workers at Delft University of Technology in the Netherlands has identified a way to push the energy and power density potentially a factor two higher. The onset of this improvement may be visible within the next five years, says Wagemaker, and will boost the use of lithium batteries in hybrid electrical vehicles.

Phase bypass

Thanks to intense R&D during the past decade, today's $LiFePO_4$ electrodes are more stable and therefore offer longer battery life than previous $LiCoO_2$-based devices. The batteries are also much safer against ignition due to overcharging, making them promising for more power-hungry applications. Modern $LiFePO_4$ batteries store lithium via a reversible first-order phase transition between $LiFePO_4$ and $FePO_4$, which is associated with a reduction in the *a*-lattice parameter. The impact of defects, particle size and charging rates on the phase transition have been intensively studied, but *in situ* X-ray diffraction experiments at the ESRF's ID11 beamline allowed the Delft team to study the chemistry of $LiFePO_4$ batteries during very fast cycling rates for the first time. This effectively allowed them to watch lithium atoms enter and exit the electrodes in real time.



Time evolution of the [200] reflection in $LiFePO_4$ electrodes from X-ray diffraction when charging rates are slow (left) and fast (right), the latter showing considerable intensity between the lithium-rich and the lithium-poor reflections.

The team found that at high charge and discharge rates, the first-order phase transition is bypassed – thereby enhancing the transport of lithium ions through the otherwise poorly conducting electrode material (*Nano Lett.* **14** 2279). "Quite against intuition, our results indicate that charging and discharging at higher rates may be beneficial for a battery's efficiency and cycle lifetime," says Wagemaker. "We have learned that the key to even faster charging is the lithium-ion transport in the electrolyte located in the pores of the electrode, which we can improve by smarter electrode designs."

The use of microbeams allowed the team to observe individual grains in the electrodes. Normally, the grains are filled one-by-one by lithium ions but the Delft results show that at higher charging rates a mixture of different lithium phases can exist within the same grain, leading to more rapid nucleation and thus charging rate. "We initially were surprised that only a small fraction of the electrode is doing this – moving like a wave through the complete electrode," says Wagemaker. "But it makes perfect sense if you realise that the lithium-ion conduction in the pores of the electrode is rate-limiting."

Understanding what's happening chemically inside a battery is the first step towards industrial optimisation, explains ID11 beamline scientist and co-author Jonathan Wright. "For applications you want to cycle batteries as fast as possible, and the ESRF gives you unique insights into that," he says. "Recharging rates are a huge issue for applications, especially for cars, plus there are applications in renewable-energy storage."

Scaling up

The Delft group is also using the ESRF to study lithium-air devices, which are described as the "holy grail" of batteries on account of their very high theoretical energy density. Commercialisation is far away, admits Wagemaker, but recently, his team performed microbeam diffraction at ID11 to investigate the fundamental processes and therefore bottlenecks in lithium-air systems.

According to chemical engineer and ESRF user Paul Shearing of University College London, who was not involved in the study, the high penetrating power of synchrotron X-rays and their ability to probe materials *in operando* can significantly speed up the application of new battery materials. "Much of the original R&D in lithium-ion batteries was geared towards consumer electronics, but there are a lot of challenges in scaling up to automotive applications," says Shearing, who has used the ESRF's ID15 beamline to image batteries. "Studies such as this are therefore very welcome."

Matthew Chalmers

Right time, right place

Chair of the ESRF's Accelerator Programme Advisory Committee, **Dieter Einfeld**, describes the quest for an ultimate light source and explains why ESRF UP PII is vital for European science.

Dieter Einfeld has spent his 40-year-long career as an accelerator physicist trying to maximise both the brightness of synchrotron X-ray sources and the number of beamlines that they can host. His track record is impressive. Einfeld designed several leading light sources including BESSY I, ANKA, SESAME, ASP and ALBA, as well as the proposed machines ROSY and LISA, and he is currently working as an expert for MAX IV in Sweden. Einfeld's lattice calculations also underlie Sirius in Brazil and major upgrades currently planned for the ESRF, APS and SPring-8.

To reach a high-brilliance machine, he explains, you need a large number of bending magnets. But in order to fit a large number of straight sections for insertion devices the machine has to be sufficiently compact to leave space for the magnets, cavities and diagnostic elements. Furthermore, since modern synchrotron users demand that the beam be stable to within hundreds of nanometres, you need a large dynamic aperture energy acceptance and closed orbit correction. "All this depends upon the arrangements of the magnets in an achromat," says Einfeld. "Each machine is unique because the available budget determines a storage ring's circumference."

Dieter Einfeld in brief

Born: 1941, Ratekau, Germany.

Education: Engineering degree, Wedel School of Engineering (1964); physics degree (1968) and PhD (1974), Technical University Berlin.

Career: Research engineer, Osram (1964–65); scientific assistant (1969–74) and research fellow (1974–83), PTB; professor, University of Applied Sciences Ostfriesland (1984–present); professor, University of Freiburg (1996–2001); technical director ANKA (1996–2001); technical director, SESAME (2001–04); head of accelerator division, CELLS (2004–12); member of the MAX-IV team (2012–present).

Family: Married, two children.

Interests: Classical music, history, walking.

> **"It would be bizarre if Europe fell behind the US."**

Engineering science

Einfeld views himself as part engineer, part scientist. On finishing high-school he took up an apprenticeship as a toolmaker before embarking on an engineering degree, during which he decided that he also wanted to study physics. He was a synchrotron radiation user from the beginning of his career, having worked on the calibration of deuterium lamps during the mid-1970s using the first-generation synchrotron X-ray source at DESY in Hamburg. At that time, he says, he and others were fighting for a dedicated synchrotron light source in Germany. "That process finished with the approval of BESSY I, and I was invited by the project's technical director to design the new source."

Two other dedicated synchrotron radiation sources were under design at the time (SRS and NSLS). But BESSY I ended up being based on a novel triple-bend achromat that bends electrons more gradually around the storage ring and therefore reduces the horizontal spread (emittance) of the beam.

In around 1990, while working on the accelerator complex at ELETTRA, Einfeld realised that the multi-bend achromat design could bring an "ultimate" X-ray source within reach: a storage ring with an emittance reaching the X-ray diffraction limit. Although it was long known that the emittance decreases with the number of magnets in the ring (to the third power), Einfeld says that there simply was no demand at the time for such extreme performance. When he asked one of his students to carry out some studies for such a diffraction-limited source, however, he was astonished by the outcome.

"With a circumference of roughly 400 m and 12 achromats one could build a machine with an emittance of 0.5 nm rad, which is roughly 10 times smaller than third-generation light sources," says Einfeld. "So discussions started about fourth-generation light sources, and 10 years later MAX-lab started to make a detailed design of such a machine based on these ideas."

Ultimate synchrotron

The proposed ESRF Upgrade Programme Phase II (UP PII) follows in MAX IV's footsteps, based on a hybrid multi-bend achromat that would produce an even smaller horizontal emittance of 0.15 nm rad. The larger-circumference APS, meanwhile, is being considered for an upgrade that would get down to 0.07 nm rad. For comparison, the diffraction limit for 10 keV X-rays is around 0.01 nm rad. There are also proposals, for instance for PEP-X at SLAC, to go further towards a diffraction limited light source.

These developments will change the global light-source landscape, says Einfeld. "It is more or less a catastrophe if ESRF UP PII does not go ahead, since Europe would lose its leading role in synchrotron radiation science," Einfeld told *ESRFnews*. "It would also be bizarre if Europe fell behind the US given that the APS upgrade is based on the ESRF UP PII lattice."

Einfeld, who in his role as chair of the Accelerator Programme Advisory Committee will help make the case for ESRF UP PII to Council, is clearly enjoying seeing his lattice ideas being turned into reality. Indeed, other than having a publication rejected while he was a PhD student, he does not recall any low points in his career. "I'm pretty lucky," he says. "I had a lot of high points and I also managed to meet the right people at the right time and in the right place."

Matthew Chalmers

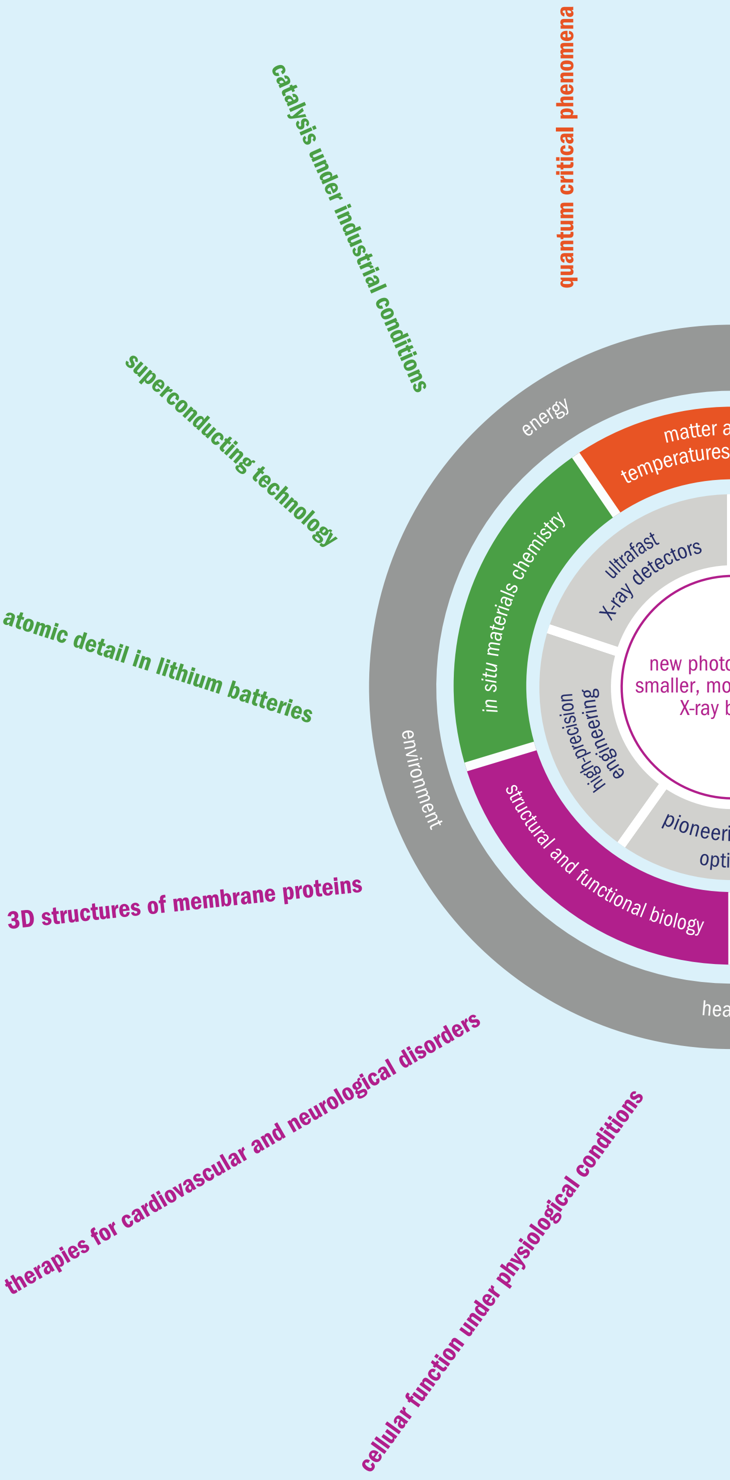
Pushing the bounda

The technical design study for Phase II of the ESRF Upgrade Programm
major 21st-century scientific challenges and for maintai

Since the ESRF entered operation 20 years ago, the brightness of synchrotron X-ray sources has increased dramatically thanks to improvements in accelerator physics and technology along with better beamline instrumentation. This has translated directly into smaller beam sizes, allowing users to reveal the structure and behaviour of matter at shorter length and time scales. Improvements made during Phase I of the ESRF upgrade will soon offer beam sizes spanning seven orders of magnitude – from 100 mm to 14 nm – with unsurpassed parallel collimation.

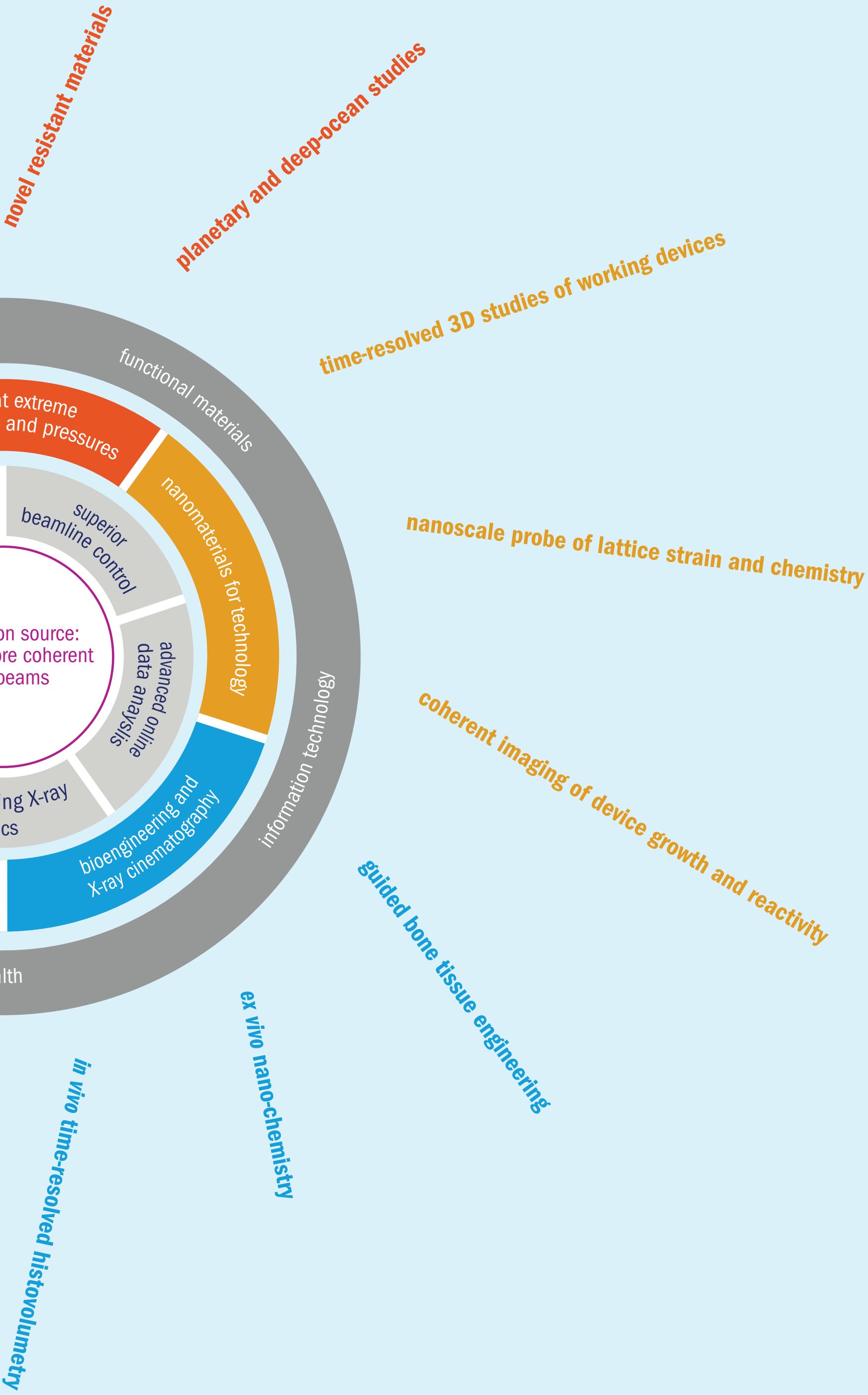
Like many of the world's leading X-ray sources, however, the ESRF is currently seeking to push its performance further to meet user demand in the decades ahead. The goal of ESRF UP PII, which is centered on a new storage ring lattice, is to boost the X-ray brightness and thus also transverse coherence. Since coherent scattering carries information about the micro- and nano-structure of materials below the size of the probing beam, the unmatched coherence properties of the new source – representing a factor 40 improvement over current levels – will open new areas of synchrotron science.

Such a machine will allow users to investigate matter and its dynamical properties from the scale of single atoms all the way up to real devices. Although smaller beams and coherent scattering techniques such as ptychography and coherent X-ray diffraction imaging have already made great strides at the ESRF, the new lattice will help address the next big challenge: to develop new methodologies for characterising embedded nanoscale structures down to the atomic level within multiscale structural hierarchies.



ries of X-ray science

e makes it clear why a brighter X-ray source is vital for addressing
ining Europe’s leading role in synchrotron science.



Core science drivers
The five main science drivers of the ESRF upgrade, which are summarised in the following pages of this issue, are intimately linked to the major societal challenges faced by Europe today: progress in biology and the life sciences has direct impact on human health; *in situ* materials chemistry is key for energy-related technologies; nanoscience and technology are at the heart of information technology; and the understanding of matter at extreme conditions provides opportunities to develop new high-performance materials. Such capabilities will also help drive European industry.

Realising the enormous scientific potential of the renewed ESRF source demands new scientific instrumentation, such as ultrafast detectors to help deal with the effects of radiation damage induced by more intense and focused X-ray beams. Advanced instrumentation – ranging from photon beam transport and sample manipulation to the analysis of large quantities of raw data acquired in a very short time – will also unlock new scientific competencies. For instance, new beamlines for serial synchrotron crystallography or hard X-ray diffraction microscopy will provide deep insight into materials and their properties that is not available today.

The ESRF UP PII technical design study, which was submitted to ESRF Council in June, lays out the full scientific and technical case for the project. If approved, work would begin next year with the new source open for user operation in 2020.

Harald Reichert, ESRF research director

Next-step source measures up

ESRF UP PII envisions the design, procurement, assembly, installation and commissioning of a new low-emittance storage ring for Europe with record brightness and coherence.

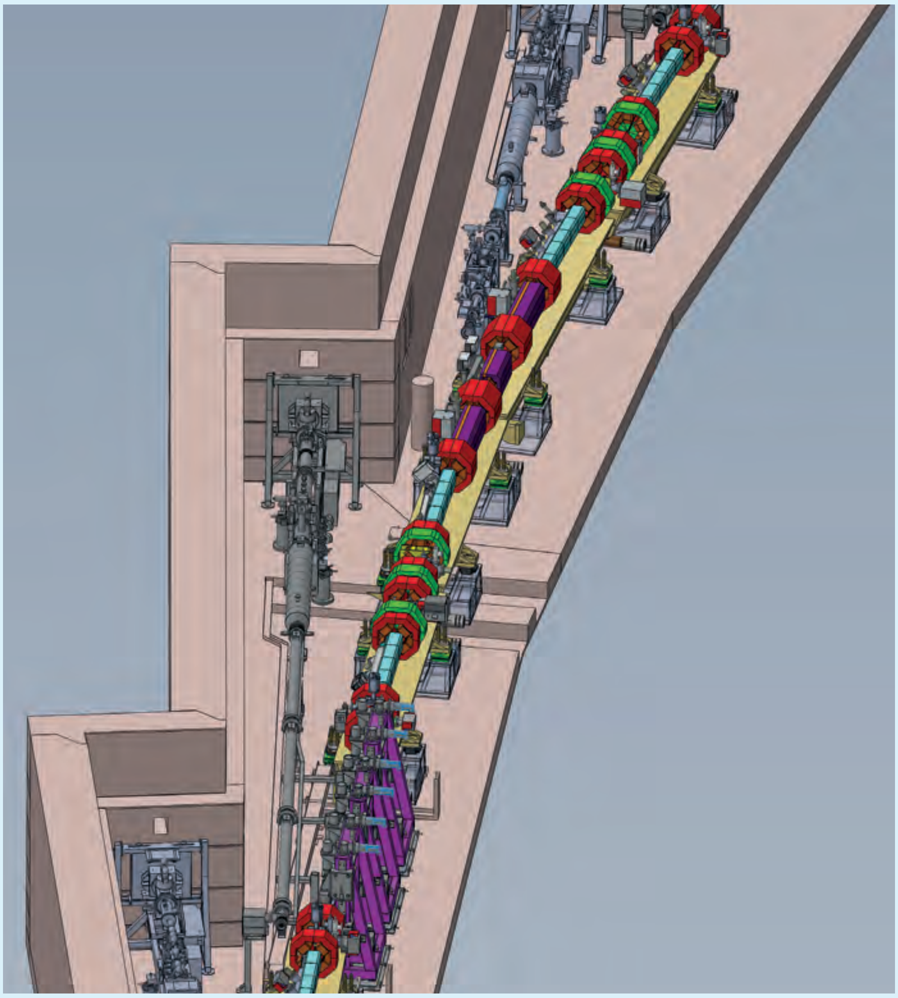
In the synchrotron world, the last decade has been characterised by a global effort to design and eventually build an "ultimate" storage ring for X-ray science. The machine would have an equilibrium emittance – a measure of the horizontal spread of the electron beam – of the order of 10 pm rad for 10 keV X-rays, which is roughly the X-ray diffraction limit. Such a storage ring would produce beams with the highest brilliance possible, and a much higher degree of transverse coherence. It is generally acknowledged, however, that a diffraction-limited storage ring would require a green-field site and is at the limit of current technologies.

The ESRF has therefore pursued an alternative strategy based on proven technologies. This creates a less ambitious project – a machine with an emittance of around 100–150 pm rad, compared to 4 nm rad for the existing ESRF lattice – but one that is readily applicable with a good cost-benefit ratio. In addition to the MAX-IV facility in Sweden, it is reasonably expected that the next decade will see up to three facilities upgraded in this way, offering users unique R&D opportunities during the next decades.

X-ray enhancement

The ESRF has long been one of the world's most brilliant photon sources. Phase I of the Upgrade Programme has already seen the performance of the storage ring, booster and linac increased beyond even the most optimistic expectations at the time of their design. Crucial developments include: enhanced beam position diagnostics providing higher beam stability and reduced vertical emittance; longer straight sections with space for additional undulators; a new and more modular RF power source based on semiconductor technology; improved RF cavities with higher-order-mode damping; and improved control systems across the source and beamlines. Taken together with the new and refurbished beamlines, ESRF UP PI offers users completely new X-ray microscopy, imaging and nano-crystallography applications.

If approved, ESRF UP PII will deliver a fully renewed facility that is capable of addressing the most challenging X-ray science questions while also delivering breakthroughs in detectors and big-data infrastructures. The proposed project is centered on the design and implementation of a new low-emittance storage ring to be constructed and commissioned in the existing tunnel, replacing the present one. ESRF UP PII would be implemented during the period 2015–2020, followed by the construction of four new state-of-the-art beamlines, and would take full advantage of new magnet design, innovative vacuum technology, beam monitoring and orbit feedback systems and other accelerator technologies that have occurred over the last 20 years at the ESRF and other facilities. These new capabilities and technologies, which were not available when the present ESRF storage ring was conceived, provide a solid basis for realising a considerably more advanced storage ring design that will maintain Europe's pioneering role in synchrotron and accelerator technologies. Such a machine is also an intermediate and necessary step in the creation of an ultimate storage ring. ●



In focus: the hybrid seven-bend achromat

The ESRF has developed a novel hybrid multi-bend achromat lattice design with a horizontal emittance of about 150 pm rad – which is roughly 30 times lower than is provided by the ESRF's current double-bend achromat lattice, with corresponding increases in X-ray brilliance and coherence.

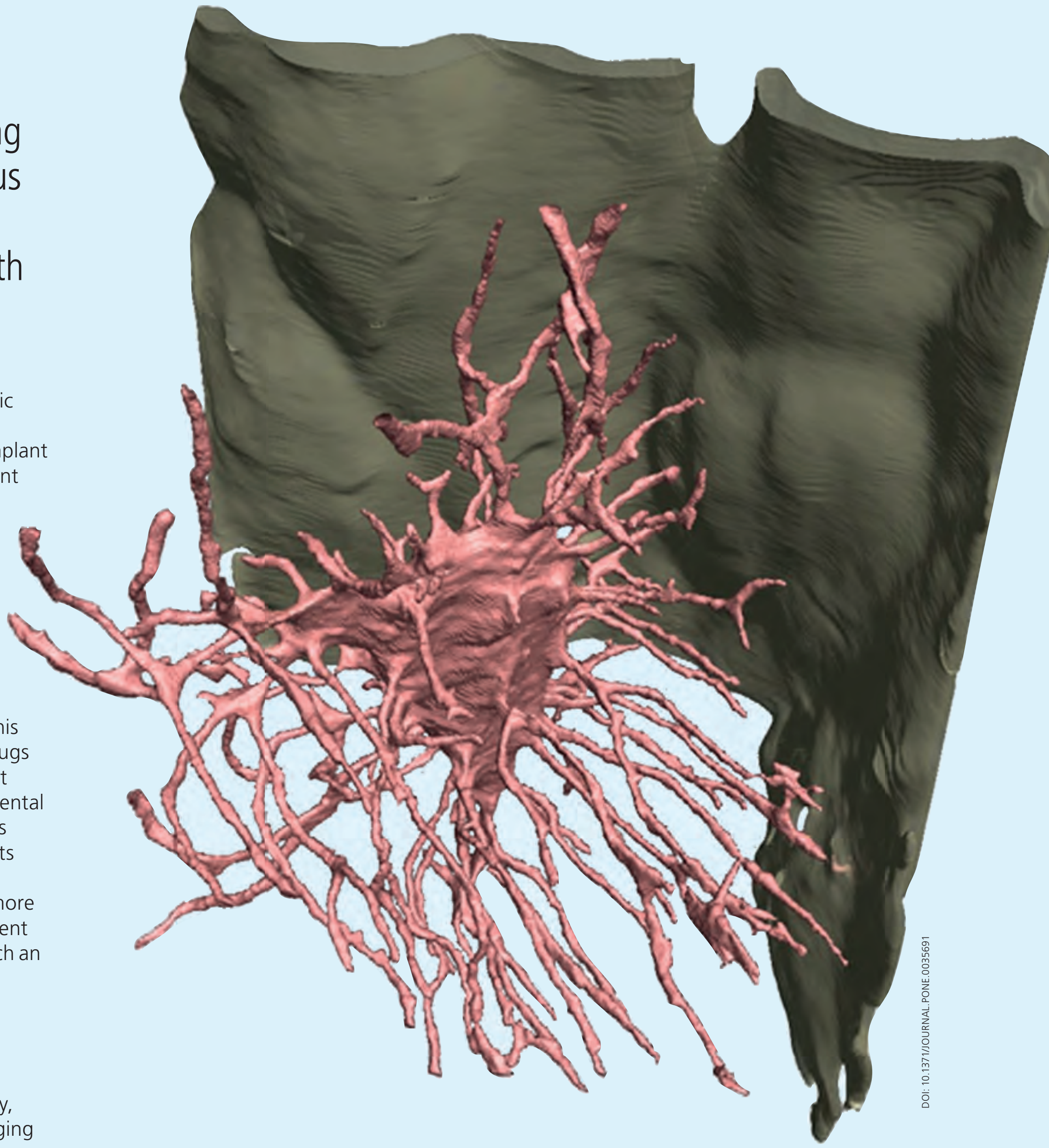
The lattice produces a small emittance thanks to stronger focusing, lower field dipoles and dipoles with quadrupolar components, with seven bends and 33 individual magnets in each of the machine's 32 cells (dipoles shown in blue, quadrupoles in red and sextupoles in green). This configuration also reduces the energy-loss per turn by around 50%, resulting in considerably lower operation costs due to decreased electricity consumption.

The new lattice, the design for which is complete, would replace the existing storage ring whilst maintaining its circumference, periodicity and beamline positions.

X-ray cinematography

Modern medicine increasingly relies on the interaction between living organisms and exogenous materials, demanding imaging at multiple length and time scales.

The fusion of biological and synthetic materials is heralding a new era in medicine. Last year saw the first implant of an artificial heart plus the development of anti-cancerous nano-capsules, while the growth of artificial organs, guided bone-tissue engineering, the use of nanoparticles in radiography are all shifting from R&D to pre-clinical phases. It is therefore vital that researchers have the necessary tools to perform full life-cycle analyses of complex systems that combine living organisms with exogenous materials. This does not only include biomaterials or drugs intentionally introduced to the body, but accidental interactions due to environmental pollution or the uptake of nanomaterials that are finding increased use in products such as cosmetics and fertilisers. The harmful effects of asbestos, CFCs and more recently PIP breast implants, are prominent examples of what can happen when such an understanding is lacking.



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X-ray phase nanotomography reveals the 3D organisation of the lacuno-canalicular network in human bone tissue. A brighter X-ray source would allow advanced *in vivo* imaging of biological systems.

Friend or foe

Although exogenous materials can be relatively simple, the body's response to them is intrinsically complex. Accordingly, we need highly versatile, multiscale imaging capabilities to follow endogenous and exogenous components simultaneously. The ESRF's X-ray imaging beamlines offer unique instruments for studying complex systems, ranging from soft materials such as proteins and cells to hard materials such as nano-electronics and catalysts, at different lengths and time scales.

Presently, the ESRF's X-ray beams can be tailored to cover a field of view as large as 10 cm with lateral resolutions reaching the nanometre scale, although not necessarily on the same experimental station. The new source, combined with the existing beamlines, will allow consecutive characterisation of the same system over several length scales. Such multiscale characterisation is simply not possible using other laboratory-based techniques, revealing morphological and chemical changes at scales approaching a single atom.

The main benefit for X-ray imaging offered by ESRF UP II is the increased photon coherence, especially at higher energies. This reduces data-acquisition times and enhances the sensitivity of phase-contrast imaging techniques, enabling scientists to perform X-ray cinematography even for dose-sensitive samples. The increased brilliance will also allow users to produce high-resolution images from structures buried deeply within an object.

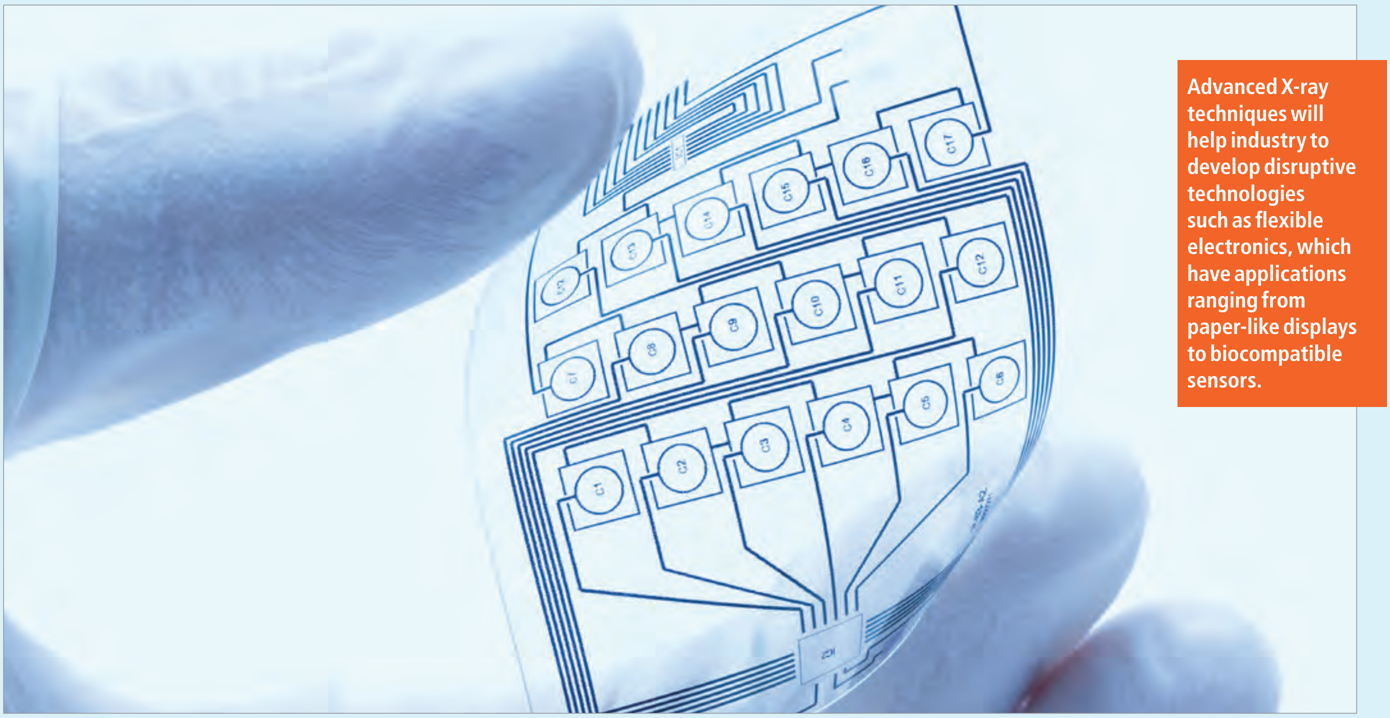
Multiscale characterisation, nanometre resolution and high penetration depth are unique properties of X-ray imaging that will greatly benefit from the improved synchrotron source. Such a source will also provide new insight in areas such as micro- and nano-technologies, applied industrial research, life sciences and energy research. The great potential of time-resolved X-ray imaging will bring processes into view across all time scales, allowing us to chart the growth of an embryo, observe a rabbit lung while breathing, or track a spinning nano-needle in an assembly of semiconductor nanostructures. ●

New opportunities

- Unprecedented characterisation of the body's response to exogenous materials;
- Multiscale analysis of heterogeneous materials;
- Low-dose *in vivo* tomography of living organisms.

Nanomaterials for technology

The ability to study the chemistry, strain and other material properties at the nanoscale will allow researchers to develop next-generation microelectronics and solar cells.



Advanced X-ray techniques will help industry to develop disruptive technologies such as flexible electronics, which have applications ranging from paper-like displays to biocompatible sensors.

Our lives have been transformed by the advent of modern high-tech devices. The smartphones that we carry in our pockets are a portal to all human knowledge, while microprocessors govern our transport, utility and communication systems. Despite these advances, many aspects of human life can still be improved. Smart houses could regulate heating and lighting or offer improved security, at the same time drastically cutting energy consumption. Self-driving cars would revolutionise transportation by offering better safety and efficiency, and smart medical devices will become increasingly important to maintain quality of life among our ageing population.

The microelectronics revolution is the result of a trend called Moore's law, which for the past 40 years has seen the number of transistors on a silicon chip double roughly every 24 months. But fundamental quantum-mechanical barriers in semiconductor architectures and difficulties in controlling thermal power dissipation mean that this growth cannot continue indefinitely. Indeed, microprocessor clock speeds have been stagnating for almost a decade.

A parallel approach to increase device performance is to make them more functional and to increase the interaction between digital electronics and the environment, for instance by combining silicon technology with high-performance III-V semiconductors to create completely new devices or radical improvements of existing ones. This hybrid "more than Moore" approach is a key element of the European semiconductor industry's strategy.

New opportunities

- *In situ* imaging of strain and chemical composition in biocompatible sensors;
- Device imaging and failure analysis under operating conditions;
- 3D imaging of nano-electronic building blocks.

More than Moore

The number of chemical elements in devices has increased dramatically in the past few years in an attempt to keep Moore's law on track, and nanotechnology is set to play an increasingly vital role. Extreme mechanical forces can be concentrated in tiny devices, for instance, inducing elastic strain that alters the atomic bonds and allows for the control of charge carrier mobility and energy bandgaps in a material. Meanwhile, the efficiency of solar cells can be improved by strain-induced bandgap tuning or by nanoparticles that offer a more efficient conversion of sunlight.

Synchrotron X-rays are a unique tool for elucidating the link between the structure of materials and their properties, and the proposed upgrade of the ESRF source will allow such methods to be applied on the much shorter length scales necessary to develop next-generation devices. Because of their penetrating power, X-rays are perfectly suited to image devices as a whole or to look at buried layers of a particular material during processing or even during operation.

Scanning X-ray diffraction techniques at the ESRF are presently able to measure the chemistry and lattice strain in samples in their native state at a resolution as low as 50 nm, but a brighter and more coherent X-ray source would offer a resolution of a few nanometres. This is crucial if we are to integrate a greater variety of materials into chips and attain a higher degree of 3D chip integration. It will allow smaller device structures to be studied *in situ* on time scales compatible with industrial experiments. The multi-modal potential of X-ray techniques is also essential to develop flexible electronics based on combinations of organic and inorganic thin films. Meanwhile, a more detailed understanding of the microstructure and defects in materials will help overcome the technical challenges of even more advanced technologies such as quantum computers. ●

In situ materials chemistry

Experiments that provide information on length scales ranging from chemical bonds to macroscopic devices under industrial conditions will drive research in energy and catalysis.

ESRF UP PII would help researchers develop the high-voltage electrodes needed for an interconnected green energy grid based on superconducting technology.

Around 6% of all electrical power generated is wasted as heat due to losses in transmission cables, equivalent to the output of more than 400 polluting power plants in the US alone. Superconductivity, whereby a material loses all electrical resistance below a certain temperature, offers a potentially lossless solution. A century after the phenomenon was discovered, however, we have not found a way to make superconducting cables economically feasible.

Synchrotron X-rays could help overcome this problem by allowing researchers to probe nanoscale defect formation, porosity, crystal size, orientation and growth during the high-pressure and extreme heat treatments involved in the manufacturing process. Presently, such diagnostic capabilities are not available at synchrotrons because they require measurement times that are longer than the duration of the relevant physical processes. But the enormous increase in flux at the ESRF provided by the proposed new storage ring would make this and numerous other *in situ* materials–chemistry experiments commonplace.

Sustainable chemistry

Developing devices and understanding processes that will allow us to move to a greener and more sustainable economy is perhaps the greatest challenge in modern materials chemistry. Catalysts are the key enabler in 90% of chemical manufacturing processes, for instance, but the increased demand for and reduced availability of raw materials means that it is vital that catalysts operate as efficiently as possible. *In situ* catalysis is a major strand of the ESRF's research, especially concerning the link between the size, shape and redox functionality of nanoparticles and their catalytic activity in systems such as car exhausts.

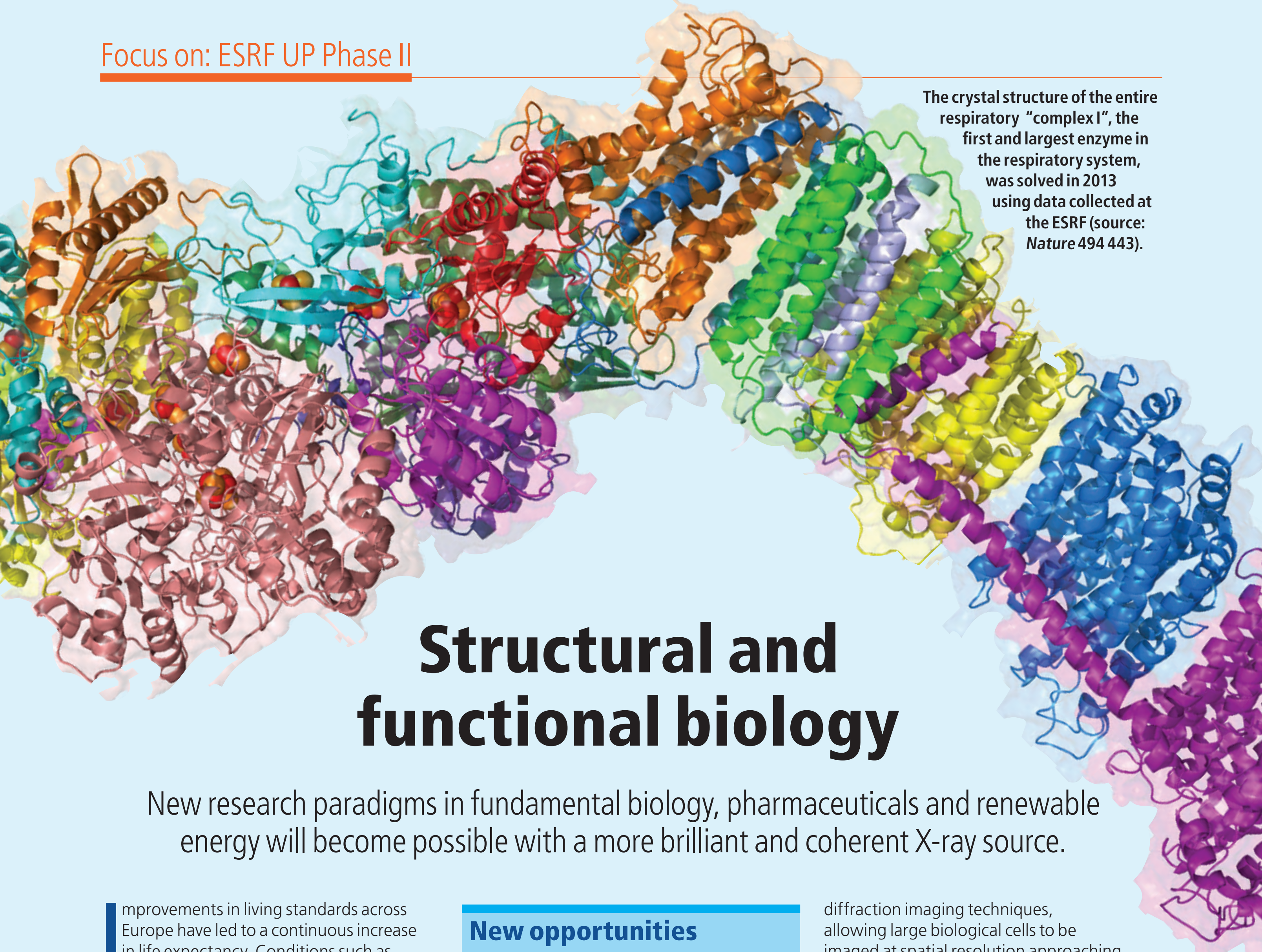
New opportunities

- Materials chemistry in devices for clean energy provision;
- Chemically resolved studies of working catalysts and devices;
- Understanding and optimising complex samples on realistic time scales.

Although synchrotron X-ray scattering and spectroscopic techniques provide atomic level detail about materials at increasingly high resolution, measurements are rarely performed under fully realistic operating conditions. In order to move from "bottom up" materials chemistry to market-ready products we need more powerful tools that can characterise complex heterogeneous systems on multiple length scales during realistic time scales and in 3D. The higher brilliance of the upgraded source would allow time-resolved 3D characterisation and the study of much faster chemical processes, representing a tremendous leap towards the study of industrial processes on full-size industrial materials.

Among the biggest opportunities are *in situ* studies of functioning fuel cells or lithium batteries, the combination of which is the most promising solution for all-electric automobiles that reduce our reliance on fossil fuels. ESRF UP PII would also revolutionise the study of chemical reactions in disordered, amorphous and liquid systems, and allow researchers to directly measure the structure of elusive reaction products in actual systems.

Techniques such as time-resolved diffraction microtomography will reveal the evolution of chemical species and nanoparticle size as a function of space and time. The hugely increased flux will allow us to fully unify tomography, diffraction and spectroscopy to provide time-resolved, 3D atomic detail *in operando*. ●



The crystal structure of the entire respiratory "complex I", the first and largest enzyme in the respiratory system, was solved in 2013 using data collected at the ESRF (source: *Nature* 494 443).

Structural and functional biology

New research paradigms in fundamental biology, pharmaceuticals and renewable energy will become possible with a more brilliant and coherent X-ray source.

Improvements in living standards across Europe have led to a continuous increase in life expectancy. Conditions such as cardiovascular and neurological diseases have therefore become major causes of death, with Alzheimer's and Parkinson's diseases also reducing the quality of life of individuals throughout old age. Although the triggers for these diseases are unknown, researchers can identify appropriate treatments by determining the atomic structures of the biomolecules responsible.

Structural biology using synchrotron X-rays provides important insights into a plethora of fundamental biological processes: the ESRF alone has allowed users to solve 10,000 individual protein structures. Macromolecular crystallography (MX) is at the forefront of applied medical research because it can reveal the mode of action of many drugs and their protein targets, and therefore provide structural information for rational drug design. Many interesting pharmaceutical targets are membrane proteins, in particular G-protein coupled receptors that often yield small and poorly diffracting crystals.

The highly intense, microfocus X-ray beams produced by ESRF UP PII would prove crucial in determining the 3D structures of these and other medically relevant drug targets. A more brilliant X-ray source would enable sub-micrometre X-ray beam sizes with an extremely high flux density, opening the door to serial crystallography (which allows the use of very small crystals to determine the structure of membrane proteins and large macromolecular complexes) and enable fast room-temperature data collection. A brighter source would also raise exciting possibilities for pump-probe, time-resolved experiments and studies of molecular dynamics.

New opportunities

- *Ab initio* crystal structure determination of large protein complexes and membrane proteins;
- Room temperature serial protein crystallography of microcrystals;
- High-resolution imaging of cells and protein dynamics during physiological activity.

Integrated approach

A full understanding of cardiovascular and neurological diseases requires an integrated approach based on MX and other techniques such as X-ray fluorescence microscopy, which can be used to probe the role of metal ions in neurological function for instance. The tremendous increase in the degree of transverse coherence at ESRF UP PII will also enhance existing scattering and coherent diffraction imaging techniques, allowing large biological cells to be imaged at spatial resolution approaching that of electron microscopy. The nanometre resolution of future ESRF beamlines will allow cellular-level investigations to be performed under appropriate physiological conditions to better understand molecular pathology and develop nanomedicines.

The study of certain proteins relevant to metabolism are also of direct relevance for the development of renewable energy sources based on biofuels. Efficient development of biofuels will almost certainly involve the structural study of enzymes, such as those responsible for the bioconversion of methane into formaldehyde. Similarly, by studying the metabolic pathways that allow certain organisms to survive in toxic environments we could find better ways both to detect pollutants and to make them less toxic.

The new and enhanced experimental techniques on offer from the new X-ray source – ranging from microbeam and serial macromolecular crystallography to high-resolution low-angle X-ray diffraction, coherent diffraction imaging and fluorescence spectroscopy – will arm life scientists and others with a unique tool to address some of 21st century society's most pressing problems. ●

Matter at extreme conditions

Probing the radically different behaviour of materials at high pressure and temperature is crucial for reaching a better understanding of our planet and for developing more resistant materials.

Microscopic processes in the Earth's interior such as grain deformation, chemical segregation and partial melting directly control large-scale phenomena including the Earth's magnetic field, earthquakes and volcanism.

New opportunities

- Probing structural complexity and its relation to quantum-critical phenomena;
- Imaging complex materials in the TPa regime at the nanoscale;
- Understanding the structure and dynamics of planetary interiors.

Nuclear fusion and other advanced technologies of the future rely on the design and synthesis of materials that can perform reliably under extreme conditions. Yet the influence of dislocations, interfaces, grain boundaries and domain walls on a material's strength make it very difficult to model the actual response of real materials to extreme radiation, pressure or temperature. Bridging this gap between theory and experiment would allow us to design harder and more resistant materials, or materials with unique chemical and physical properties.

Science at extremes of pressure and temperature is a vibrant international field that addresses problems in domains ranging from fundamental condensed matter physics and planetary science to material synthesis and biology. In the past two decades, research pioneered at the ESRF and other large facilities has shown that unexpected physical and structural behaviour at ultrahigh pressure is the rule rather than the exception.

These studies not only allow a better understanding of the inner structure of the Earth and giant planets in our solar system and beyond, but allow us to tackle major challenges such as the deep carbon cycle and the search for future energy sources. Extreme-conditions research is also crucial for exploring the hostile environment of the deep oceans, which are the largest yet least understood habitats for microbial life.

The TPa regime

Pressure is a powerful thermodynamic variable because it strongly alters interatomic distances without changing the thermal energy or chemical environment. Remarkably, the ESRF's high-pressure beamlines allow users to determine the structural, dynamical, electronic and magnetic properties of materials at pressures of up to 100 GPa with the same precision as is possible at ambient conditions.

The sub-micrometre-sized beams produced by ESRF UP PII would take this precision to the TPa regime, where core electrons are predicted to participate in bonding and therefore lead to complex new spatial arrangements. Furthermore, the increased coherence of the X-ray beam at high energies will allow phase-contrast and other coherent imaging techniques to pinpoint morphological, strain and chemical states at a resolution of a few tens of nanometres and will open the study of dynamical phenomena such as phase transitions and melting.

By extending these studies to include pulsed magnetic fields as a variable, users would be able to explore the interplay between superconductivity and structural order, for instance. The combination of magnetic fields with high pressure and low temperature, meanwhile, would provide an ideal test bench for quantum-critical phenomena such as in new spin structures of anti-ferromagnetically coupled sublattices. The higher brilliance of the upgraded X-ray source would also probe the liquid phase at pressures that are not currently accessible to detailed structural studies, such as dense CO_2 and supercritical fluids.

Exploring even greater extremes of density and temperature will require moving from the static to the dynamic regime, based on compact high-power lasers. Measurement times as short as 0.1 ns will provide an ideal way to study the exotic state called warm dense matter and will complement research at X-ray free electron lasers and other facilities in the rapidly advancing field of extreme matter. ●

The ESRF can help the chemical industry seek more efficient and more environmentally compatible processes for the manufacture of raw materials.

New source widens industry appeal

Creating industrial impact is part of the ESRF's mission. ESRF UP PII will help enable new industrial partnerships in microelectronics, biotechnologies and new materials.

Above and beyond the established long-term benefits of curiosity-driven research, European governments desire more direct economic returns from their investments in large research infrastructures. Companies are becoming increasingly important users of facilities such as the ESRF, with specific service needs. To a large extent, as the first third-generation light source, the ESRF has set the scene for modern industrial synchrotron use. Today, an estimated 20% of all ESRF experiments involve collaborations with industrial R&D centres and 40% of users state that their work has industrial applications.

Industry researchers need ever finer analysis tools both to undertake the most demanding proprietary research and when carrying out pre-competitive R&D. A more brilliant X-ray source at the ESRF would also continue to drive the European instrumentation industry, worth €4–5 bn annually. The Phase II upgrade will require significant leaps in X-ray optics, high precision mechanics, magnet assemblies, vacuum technologies and other high-performance tools for both academic science and industrial R&D, generating rich opportunities for European industry collaborations.

New opportunities

- Nanoscale characterisation of materials;
- *In situ* studies of systems under processing conditions;
- Advanced software and automation for high-throughput industrial materials characterisation.

> **"The ESRF has set the scene for modern industrial synchrotron use."**

Priority research

At the heart of industrial R&D challenges today is the understanding of novel materials, be they smart, nano-structured, biodegradable, manufactured energy-efficiently or sustainably resourced. Advanced synchrotron X-ray tools can enable companies to put such materials into use, and the nanoscale beams from an upgraded ESRF source will allow researchers to look inside materials and devices under increasingly process-relevant conditions.

ESRF UP PII will further broaden the reach of the ESRF, going beyond the traditional pharma and biotech industrial user-base for protein crystallography, to nano-characterisation in physical and materials science, such as next-generation electronics and catalysts. It also includes plans for more streamlined and automated software to provide high-throughput, robust data pipelines, following the successful model already demonstrated in protein crystallography.

The ESRF is open to ideas about how its new facilities can meet industry interests, for instance by creating industry-specific instrumentation on beamlines as has successfully been demonstrated at other light source facilities and by delivering data that has been analysed to make it more understandable to non-expert users. There is also scope for partnerships in targeted areas such as advanced detector sub-systems and high-speed electronics, and its spillover to high-end imaging applications. An upgraded X-ray source will maintain the ESRF's leading role in Europe as a hub for high technology, innovation and training. ●

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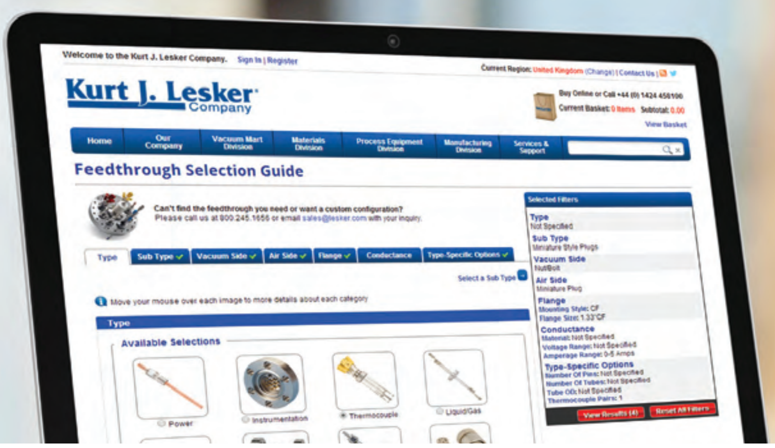

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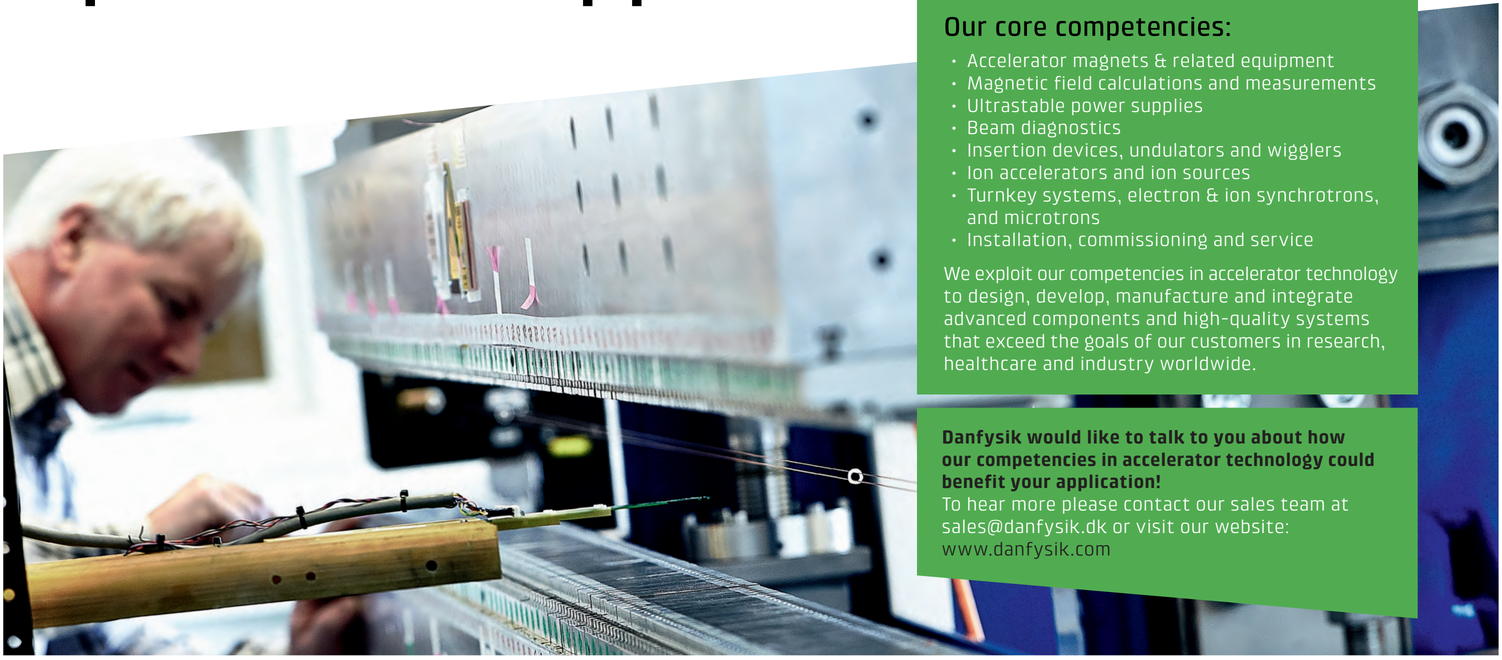

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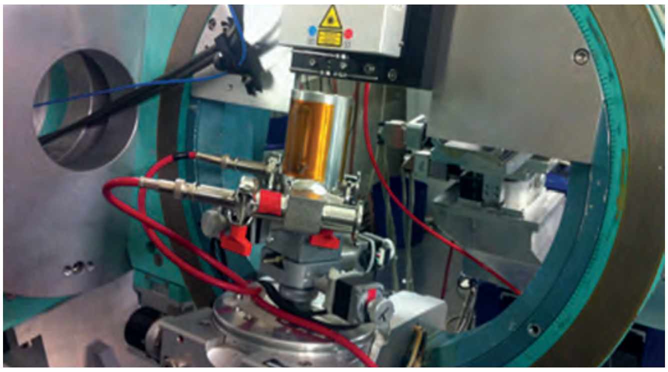
XMaS takes the strain off Moore's law

The ESRF's XMaS beamline is helping IBM and other electronics companies develop piezoelectric transistors that are faster and less power hungry than existing devices.

For the past 10 years, computer clock-speeds have flat-lined, marking the demise of a 40-year-old trend known as Moore's law. This trend has seen the dimensions of individual devices in integrated circuits halve every two years or so, with a corresponding increase in processing ability. But with transistor gate lengths now measuring a few tens of nanometres, yet switching-voltages remaining at the 1V level, we are close to the limit of silicon CMOS technology due to the difficulty in extracting heat from devices.

Piezoelectric transistors are seen by IBM and others as one of the most promising ways to get Moore's law back on track. Simulations show that clock-speeds 10 times larger than today's CMOS equivalent are possible by using a small voltage to switch small regions of piezoresistive materials between an insulating and conducting state – a process that also consumes 100 times less power than today's CMOS transistors, studies show. In 2012, IBM researchers developed the first piezoelectric-effect transistor, but the challenge now is to find out if these attractive features are scalable to the dimensions of CMOS devices.


NPL/XMAS

Interferometer and sample holder on the XMaS Huber diffractometer during commissioning in February 2014 as part of the Nanostrain project.

Nanostrain is a three-year, €4 m project funded under the European Metrology Research Programme (supported by the EC and EURAMET) to characterise strain at the nanoscale under industrially relevant conditions. Involving Europe's leading metrology laboratories and companies including IBM and ST Microelectronics, the success of the project relies on new synchrotron X-ray techniques under development at the ESRF's UK-operated XMaS beamline.

Promising results

The aim is to combine X-ray diffraction, which is routinely used to measure the atomic periodicities in crystalline materials, with laser interferometry, which is able to measure extremely small displacements in bulk materials. This will enable the team to link intrinsic displacements due to changes of the unit cell's size and ionic movements, with macroscopic changes that typically are also due to extrinsic phenomena such as defects and domain-wall motion. "The main challenges are sensitivity and noise levels, so we have developed an interferometer mount to create a rigid and stable system," explains Tom Hase, co-director of Warwick University in the UK.

Members of the Nanostrain team from the UK's National Physical Laboratory carried out the first tests of the new tool at the ESRF in February this year – with promising results. "During the first commissioning time we measured the displacement on a piezoelectric single crystal both in static and dynamic electric fields and observed displacements of less than 1 nm, which is well within the desired range," explains Carlo Vecchini of NPL. The next goal at XMaS is to push the switching frequencies from around 100 Hz to the kHz and possibly up to 1 MHz by the end of the project, he says. "This will enable the simultaneous measurement of macroscopic displacement, electric polarisation and X-ray diffraction data in near operational conditions."

Experiments on real samples will be carried out this summer, and the advanced X-ray techniques are expected to benefit other areas of XMaS science. "The Nanostrain project has already led to advances in the ways that multiferroic materials can be studied on the XMaS beamline, and we anticipate further application of the methodologies to a wide range of material systems," says XMaS co-director Chris Lucas of Liverpool University in the UK.

Matthew Chalmers

Movers and shakers

New ESRF group heads

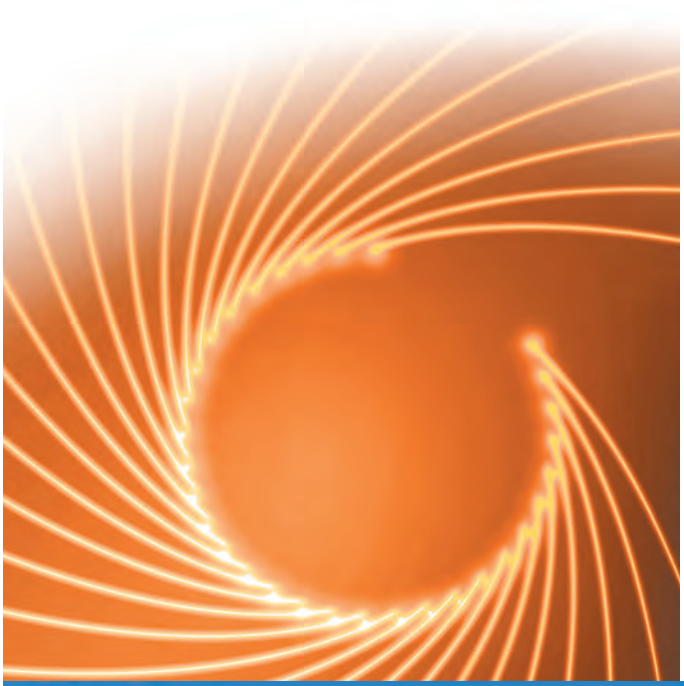
Sakura Pascarelli has replaced Nick Brookes as head of the Electronic Structure and Magnetism Group, while remaining scientist-in-charge of the XAS beamlines BM23 and ID24. Pascarelli, who trained as a physicist, joined the ESRF staff in 1997 having previously worked on the Italian CRG beamline BM08 (GILDA). Her research currently focuses on studies of matter at extreme conditions of pressure, temperature and magnetic fields using X-ray absorption spectroscopy and X-ray magnetic linear and circular dichroism.

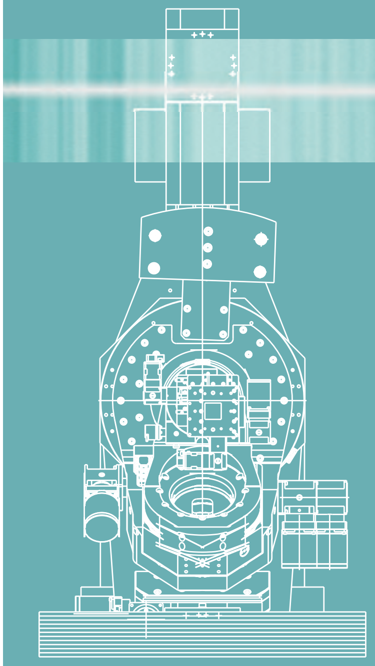
Gordon Leonard has been appointed head of the Structural Biology Group, having previously been the group's deputy head. Leonard has been at the ESRF since 1996, with research interests including LysR transcription factors and the elucidation of the crystal structures of proteins and nucleic acids at ultra-high resolution. He replaces Sean McSweeney, who has taken up a position at Brookhaven National Laboratory in the US.

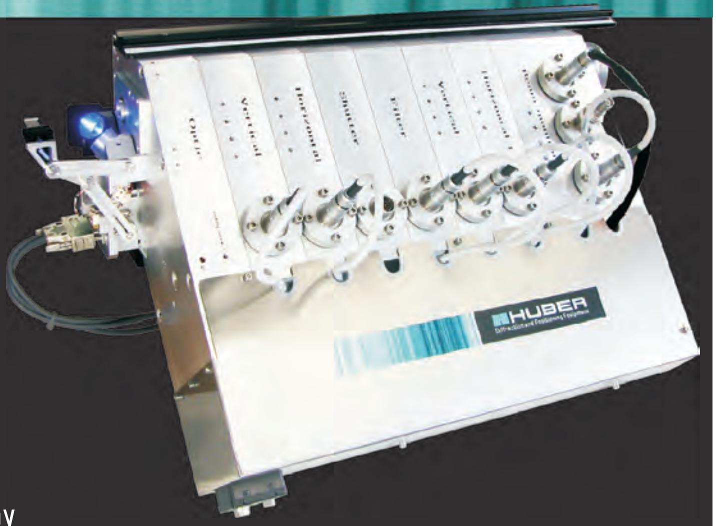
Veijo Honkimäki, previously head of the high-energy diffraction and scattering beamlines ID15A&B, has become head of the ESRF's Structure of Materials Group – which includes ID15 and five other beamlines plus associated facilities. Honkimäki, who previously was deputy head of the group, joined the ESRF in 1995 and works in the area of materials science. He replaces Roberto Felici.

E-XFEL prepares for users

One of the first ESRF staff members, **Silvia Bertini**, has been appointed head of the User Office at the European XFEL in Hamburg, Germany – a newly created position in preparation for the facility's first user operation in 2017. Bertini took up a secretarial post at the ESRF in 1991 and then worked in the Office of the Directors of Research between 1994 and 2004. Following a move to the Administration team of EMBL Hamburg, Bertini joined the European XFEL in 2012.



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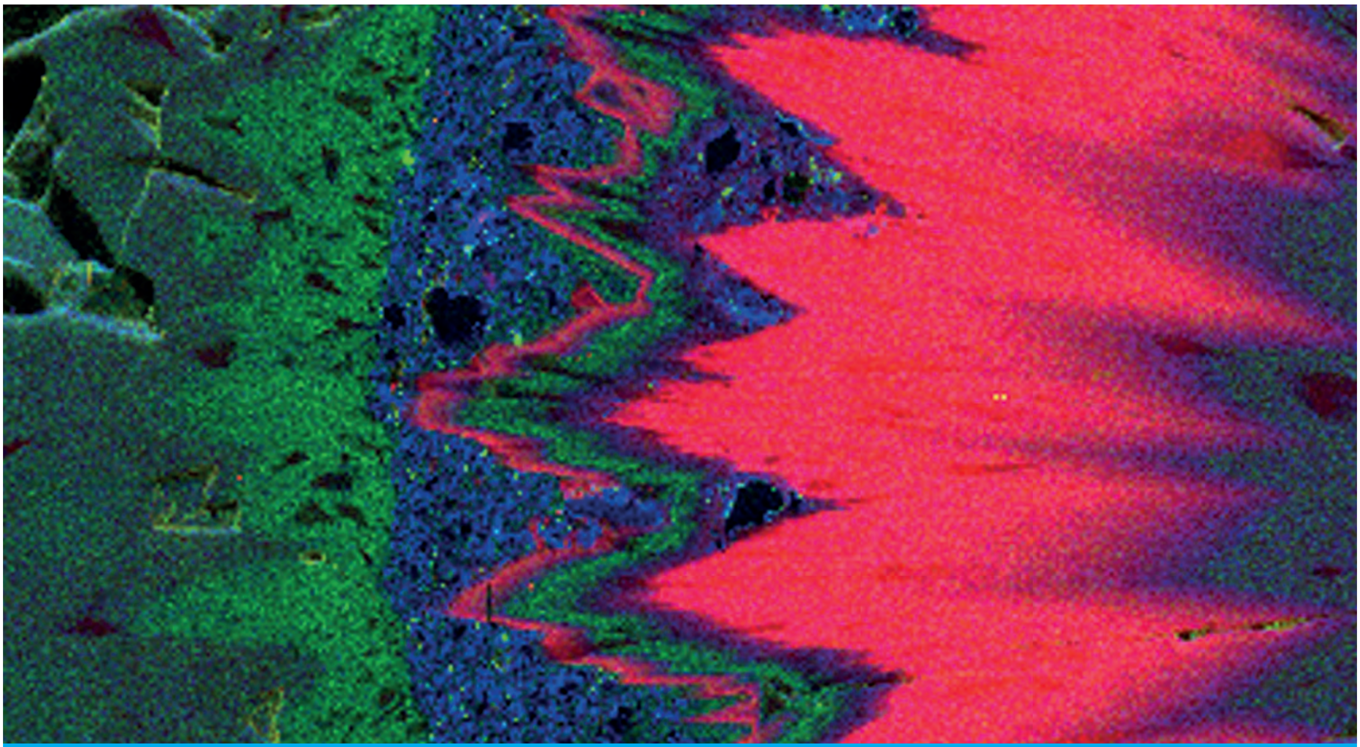
Beauty of science



Ice work: This synchrotron µXRF map reveals the complexity of subglacial environments in the East Antarctic Ice Sheet during the last glacial maximum 27,000–17,000 years ago. Obtained from polished slabs of calcite formed beneath the ice, the panel represents a region 2 × 0.8 mm and shows the presence of sulphur (red), phosphorus (green) and magnesium (blue). The study, which was carried out at the ESRF's ID21 and ID22 beamlines by Silvia Frisia of the University of Newcastle in Australia and co-workers, suggests a role for subglacial production and transport of nutrients to the Antarctic ocean, which contributed to carbon sequestration – and thus the Earth's climate – during the last glacial maximum (submitted for publication).

In the corridors

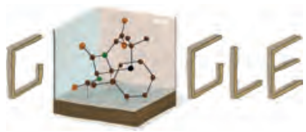
Calling all UK users

ESRF users from the UK have responded to an open consultation set up by the UK government to assess the country's involvement in large-scale research infrastructures both at home and abroad. Announcing increased capital investment of approximately £5 bn for the next five years, the government's Department for Business Innovation & Skills (BIS) sought input from the scientific community to help identify strategic priorities for long-term science and research capital investment, such as the potential ESRF UP PII. The consultation closed on 4 July and can be accessed at https://bisgovuk.citizenspace.com.

Spiders on show

Giant 3D printouts of spiders as they would have looked tens of millions of years ago are on display at a new spider exhibition at the Museum of Grenoble. Recreated from X-ray microtomography scans at the ESRF's ID19 beamline based on imprints left in amber, the magnified models reveal intricate details of the ancient arachnids – some of which were smaller than dust mites. A second display reveals how researchers use the ESRF to study spider silk in order to recreate its structure. It was at the ESRF's ID13 beamline that the first unique diffraction signal from a single silk fibre was measured: the exhibition showcases a small motor that pulled silk directly from the spider so that it could be studied *in situ*. Similar tools have since been developed for silkworms at the ESRF's DUBBLE beamline. The Grenoble exhibition received more than 5000 visitors in its first month of opening and will run until March 2015.

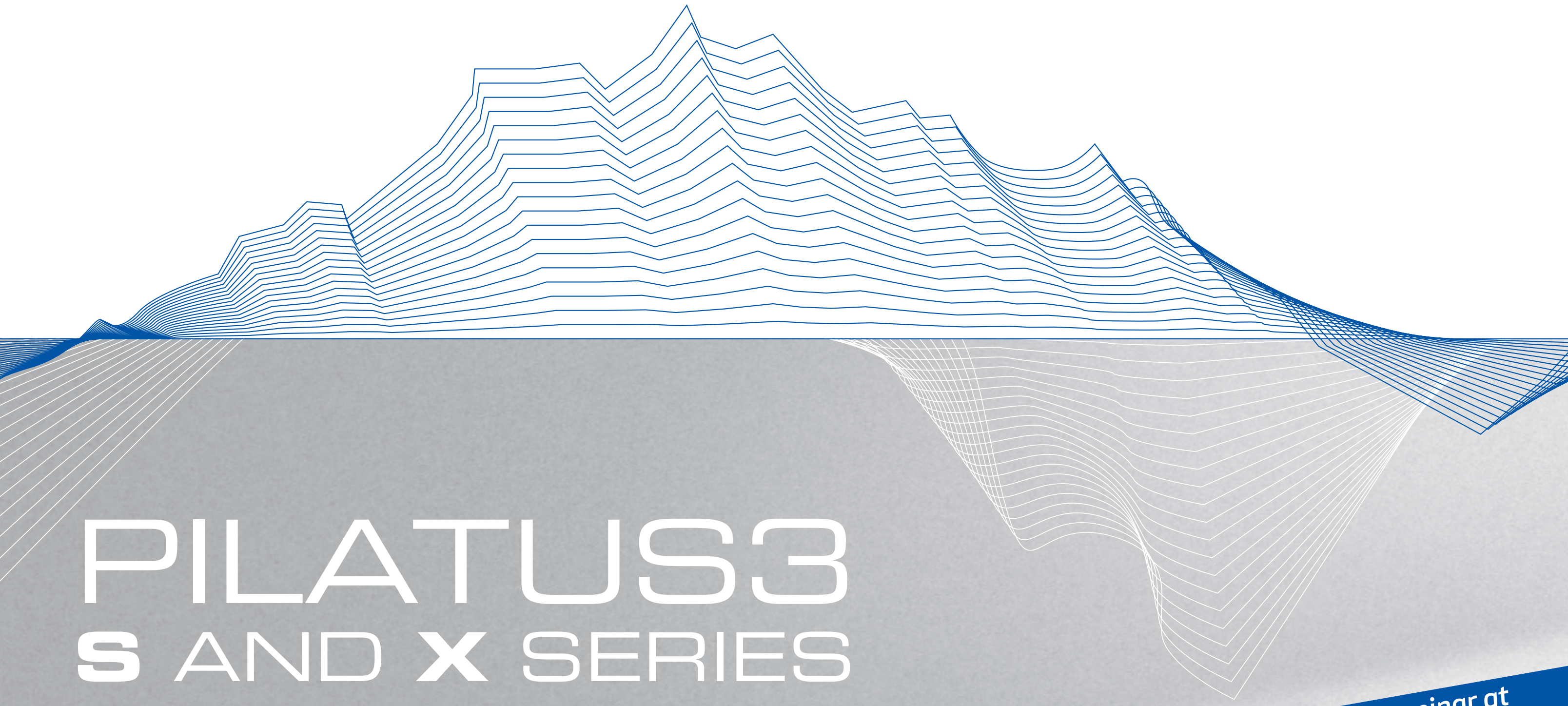
Google celebrates structure



On 12 May, marking what would have been Dorothy Hodgkin's 104th birthday, search engine Google turned its logo into a ball-and-stick model of penicillin – the structure of which was solved by Hodgkin in 1945. The pioneering X-ray crystallographer also confirmed the structure of vitamin B12, for which she became the third woman to win the Nobel Prize in Chemistry, and later cracked the structure of insulin.

LEGO puts women in science

Toy manufacturer LEGO has announced a new mini-figure set featuring a female astronomer, palaeontologist and chemist. The idea was submitted to the LEGO Ideas website by Swedish geochemist Ellen Kooijman where it passed the 10,000-vote threshold required to take the project into the design phase. Called the LEGO Research Institute, the set is due to hit the shops in autumn.

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