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ESRF looks ahead as funding difficulties of certain member states are eased

The ESRF has today the most successful and productive scientific programmes in Europe and, indeed, worldwide, with one scientific paper in Nature or Science every second week, on average. Nevertheless, the status of the European economy requires a revision of the ESRF’s programmes.

Every international research organisation must take account of the economic conditions of its member countries. Today, we at the ESRF, have put in place a temporary scheme to alleviate the exceptional funding problems of some of them. I am pleased that all 19 member and associate countries remain firmly committed to maintain, in a sustainable way, the current world leadership of the facility. Their support fuels the transformation of today’s difficulties into the opportunities of tomorrow.

This scheme, established by the Council and the management, will alleviate the present financial difficulties of Italy and the UK in funding science programmes. At its meeting on 29–30 November, the Council unanimously adopted a three-year resolution allowing these two member countries to reduce their financial contribution and, most importantly, preserving the quality of the ESRF’s scientific programme. All 12 member countries and seven scientific associates have renewed their long-term commitment to the ESRF, and especially to the continuation of its inter-governmental convention.

The approval of the resolution determines a 6% reduction in expenditure capacity over the 2011–2013 period, which will be absorbed with no compromise on the quality of service to the 5,000 scientists who use the ESRF. The expenditure shortfall will be dealt with by reducing the number of beamlines and/or operation time of the accelerator complex, along with a revision of the deliverables of the Upgrade Programme. The implementation schemes of these saving scenarios will be prepared for decision at the spring 2011 meeting of the ESRF Council.

This strategy will maintain the ESRF’s world leadership in synchrotron science, and will create new opportunities for more unique beamlines on newly available insertion device straight sections on the ESRF storage ring. Our new world record in vertical emittance allows us today to deliver the brightest high-energy X-ray beam worldwide (2 x 10^{21} photons/s/mm^2/mrad^2/0.1bw at ~40 keV), and we expect that many new partners will be interested in exploiting these new unique possibilities.

Over the next three years, we will make efforts to attract new members, scientific associates and other possible ways of collaboration with third parties interested in injecting new resources into our facility. In parallel, together with the Council, we will work to develop new schemes to finance the ESRF’s needs, which will also take into account the scientific use by a member country in determining its financial contribution.

The new times are a welcomed challenge for synchrotron science in general. The spectacular results that Europe, in particular, has achieved in the last 10 years with the construction of new excellent national synchrotron sources, highlights European leadership in this field. Today, new important investments are foreseen in the US and in Japan, and a strong programme is being developed in Russia – with its long tradition in synchrotron science – and in emerging economies such as Brazil, China and India.

We need a careful co-ordination to emphasise the complementary aspects of the ESRF with the other European sources. In order to maintain Europe’s leadership, and to open our institutes to innovation, industry and new communities, we must co-ordinate and collaborate immediately on issues such as cost containment, efficiency, excellence in user service, technical developments and governance. This is the only way, in my opinion, to ensure optimal scientific competition, throughput and opportunities for the most vigorous, numerous, growing, diversified and productive scientific community ever seen in modern times.

Francesco Sette, director general

1 Under the resolution voted by the ESRF Council, all parties retain their contractual shares and voting rights. However, instead of contributing 15% to the approved ESRF budget, Italy will contribute 13.41% and 10% respectively. These figures are likely to be maintained for the next three years. Likewise, the UK contribution is reduced from 14% to 10%. The other parties, along with the seven scientific associates, will maintain their contributions as planned. The use of the ESRF by scientists from a given country is linked to the shares held by that country with, however, considerable flexibility aimed at the exceptional funding problems of some of them. I am pleased that all 19 member and associate countries remain firmly committed to maintain, in a sustainable way, the current world leadership of the facility. Their support fuels the transformation of today’s difficulties into the opportunities of tomorrow.
Research indicates Neanderthals grew faster than humans

A multinational team of specialists, led by researchers from Harvard University, Max-Planck Institute for Evolutionary Anthropology and the ESRF, applied cutting-edge synchrotron X-ray imaging to resolve microscopic growth in 10 young Neanderthal and Homo sapien fossils. During this five-year study, the scientists found that Neanderthals’ teeth grew significantly faster than our own species, including some of the earliest groups of modern humans to leave Africa between 90–100 000 years ago.

The Neanderthal pattern appears to be intermediate between early members of our genus (e.g. *Homo erectus*) and modern humans, suggesting that the characteristic slow development and long childhood is a recent feature unique to our own species. This extended period of maturation may facilitate additional learning and complex cognition, possibly giving early Neanderthal and Homo sapiens a competitive advantage over their Neanderthal cousins.

Reference
T M Smith, P Tafforeau et al. 2010 *PNAS* doi:10.1073/pnas.1010906107

An AIDS drug could help in the fight against herpes

Herpes and AIDS have more in common than you would think. Scientists at the Institute for Research in Biomedicine in Barcelona (Spain) and the EMBL have discovered that an approved drug for the treatment of AIDS could also help in attacking the herpes virus. The family of herpes viruses includes pathogens such as, among others, the virus that causes chickenpox, the Epstein-Barr virus, associated with several types of cancer; the herpes virus, associated with Kaposi sarcoma – in AIDS patients – or the human cytomegalovirus (HCMV). Although 90% of adults carry HCMV, this virus is opportunistic, acting in people with weakened immune systems, such as in cancer and AIDS patients, recipients of organ transplants and neonates. The HCMV causes neurological defects in 1% of neonates in developed countries. It also results in retinitis that deteriorates into blindness in 25% of subjects with AIDS, defects in the brains and central nervous systems of young adults, mononucleosis and diseases of the throat.

The way that the herpes virus functions is by entering the nucleus of a cell where it uses the cell machinery to copy its DNA several times into a single large chain. Once this copy has been made, it acts as a complex called terminase, formed by three protein subunits. The terminase cuts the new DNA into small fragments, the size of a single viral genome, and introduces these into empty shells (capsids) that have developed in the cell nucleus. Then, the new viruses leave the cell to continue infection.

The researchers resolved the 3D structure of one part of the terminase using the beamlines ID14, ID29 and BM16, and when they observed that it resembled the integrase of the AIDS virus, for which drugs are available, they tested it against the herpes virus protein. The results led to the conclusion that raltegravir, an approved drug against AIDS, cancels the scissor function, which is required for viral replication. This is the first step towards the development of a drug against the entire herpes virus family.

Reference
M Nadal et al. 2010 *PNAS* 107(37) 16078–16083.

Users’ corner

Following the 1 September deadline, 947 proposals for ESRF beamtime were received. In view of possible changes concerning the rules for the allocation of beamtime and national balance, the final decisions on beamtime allocation are withheld until after the Council meeting on 29 and 30 November. Please be aware that the final decisions will therefore be sent out later than usual for this round.

The next deadline for submission of standard proposals will be 1 March 2011. The next deadline for submission of long-term proposals is 15 January 2011. Please remember that work on several upgrade beamline projects has already started and users are advised to check the availability of beamlines for future proposal deadlines by consulting our Beamline Status table at www.esrf.eu/UsersAndScience/UserGuide/Applying/beamline-status.

The plenary session of the 21st ESRF Users’ Meeting will take place on 8 and 9 February 2011. Three workshops will be associated with the Users’ Meeting:
– X-rays and neutrons in energy-related materials science.
– New developments in time-resolved studies with synchrotron radiation.
– Structure and magnetism in multiferroics.
More information about the Users’ Meeting can be found at www.esrf.eu/events/conferences/usersmeeting2011/

News from the beamlines

– *Since September the new Sample Changer system, which is able to automatically expose micro-volumes of proteins in solution with minimum time overhead, is available to users on the ID14-3 bio-SAXS beamline. Volumes of solution down to 5 µL, stored in strip wells or in micro-plates, can be automatically loaded for exposure to X-rays (in a vacuum-mounted glass capillary). After exposure, the fluid path is cleaned and dried automatically in tens of seconds. The robot can hold several hundreds of samples with a temperature control of 2–60°C and it is highly appreciated by both external and internal users.*
– *A new ultra-high vacuum (UHV) system for photoelectron spectroscopy (PES) and X-ray standing-wave measurements has been commissioned at ID32. The central part of the new instrument is a novel hard X-ray PES (HAXPES) spectrometer (PHOIBOS 225 HS from SPECS, Berlin), working up to 15 000 eV electron kinetic energy with an energy resolution ∆E/E down to 10–6. An energy resolution of 50 meV at 8 keV, i.e. ∆E/E = 6·10–6 has been achieved in first tests.* This new system replaces the old UHV chamber with the PHI electron analyser.
When the egg meets the sperm: the female side of the story

At the beginning of conception, sperm binds to proteins in the extracellular coat of the egg, called zona pellucida (ZP). But the molecular details of this fundamental biological event have so far remained obscure.

Now researchers at the Karolinska Institutet (Sweden), together with scientists from Nagoya University and the ESRF, have been able to describe the 3D structure of the receptor molecule that binds sperm, called ZP3. The results will lead to better understanding of infertility and may enable entirely new types of contraceptives.

The detailed structural information, based on data collected at the structural biology beamlines, makes it possible to begin exploring at the molecular level how the egg interacts with sperm at fertilisation. The study suggests which parts of the receptor are likely to be directly contacted by sperm, and it provides new insights into how the sperm receptor is assembled and secreted from the egg. The findings have important implications for human reproductive medicine because they may explain how mutations in the sperm receptor gene could cause infertility. Potentially the research could lead to the design of non-hormonal contraceptives specifically targeting egg–sperm interaction. “The results give a remarkable picture of the female side of fertilisation,” says Luca Jovine, who has led the study. “The next step will be to tackle the corresponding molecules on sperm that allow it to bind to the egg.”

Reference
L Han et al. 2010 Cell 143(3) 404–415.

The border of the unknown

The border between the core and the mantle of the Earth is located 2900 km under our feet. With a pressure of around 1.4 million times the atmospheric pressure and a temperature of more than 4000 K (~3900 °C), this zone is the home to chemical reactions and changes in states of matter still unknown. The seismologists who have studied this subject have observed an abrupt reduction in the speed of the seismic waves, which sometimes reaches 30% when getting close to this border. This fact has led scientists to formulate the hypothesis, for the last 15 years, of the partial melting of the Earth mantle at the mantle–core border. A team from the Institut de Minéralogie et de Physique des Milieux Condensés in Paris and the ESRF has shed some light on this hypothesis by using a new approach, employing X-ray diffraction at the high-pressure beamline ID27.

It used an X-ray diffraction technique at the high-pressure beamline ID27. The in situ laser-heated, high-temperature and high-pressure diffraction measurements allowed them to determine what mineral phases melt first. They also established, without extrapolation, fusion curves of the deep Earth mantle (i.e. the characterisation of the passage from a solid state to a partially liquid state). The team’s observations show that the partial fusion of the mantle is possible when the temperature approaches 4200 K. These experiments also prove that the liquid produced during this partial fusion is dense and that it can hold multiple chemical elements, among which are important markers of the dynamics of the Earth mantle. These studies will allow geophysicists and geochemists to achieve a deeper understanding of the mechanisms of differentiation of the Earth and the history of its formation, which started around 4.5 billion years ago.

Reference

Scientists follow metalloenzymes with X-rays

Scientists from the Commissariat à l’Energie Atomique (CEA), the University Joseph Fourier and the Centre National de Recherche Scientifique (CNRS) have been able to observe all the key steps of an essential process in life: the activation of oxygen. They have done so by creating an artificial metalloenzyme – a complex made up of a chemical catalyst and a protein.

The structure of artificial metalloenzymes consists of an inorganic catalyst inserted inside an inactive protein structure. The first one dictates the reaction in the active site of the enzyme, while the latter controls the making of the product and the effectiveness of the chemical reaction.

The research team could follow the chemical reaction in the active site over time thanks to the X-rays of the structural biology beamlines ID14, ID23 and BM30A at the ESRF.

Reference
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Increasing the fatigue resistance of fan blades

Rolls-Royce plc and the University of Manchester work together to improve the fatigue resistance of materials used in the aerospace industry. The ESRF has become an important tool in their research.

The initiation and propagation of fatigue cracks can be suppressed by the introduction of compressive residual stresses. The most commonly used method is to fire “shot” at the surface (Shot Peening), which generates compression to a depth of about 100–500 µm. In recent years, however, Rolls-Royce has introduced a new method called Laser Shock Peening (LSP). In LSP, a high-power laser pulse irradiates the surface of the material, producing plasma that generates shock waves. These induce compressive stresses on and beneath the surface. This method has the advantage that it improves the depth of compressive residual stress fields (up to several millimetres) in the material while maintaining a smooth surface finish.

Around 10 years ago Rolls-Royce was one of the first companies to use LSP commercially, applying it to aero-engine fan blades. “It is absolutely critical that fan blades resist the effect of fatigue and fretting fatigue over many thousands of flying hours,” explains Phil Withers, professor of materials science at the University of Manchester and leader of the collaboration with Rolls-Royce and the ESRF. “The University of Manchester supports Rolls-Royce in qualifying the LSP production process,” he says.

Lab X-rays require metal removal and measurement correction to determine stress profiles and are therefore destructive. The highly penetrating, non-invasive, hard X-ray beams of the ESRF come into the picture when the researchers try to understand the structural changes taking place in the fan blades during the service throughout their lives. Rolls-Royce has techniques that can simulate a very wide range of extreme service conditions. “Synchrotron radiation is the only means of characterising the way that these protective stresses evolve over the life of the component without destroying the part,” Withers explains.

At the ESRF, scientists probe the samples with a very high spatial resolution on beamlines like ID11, ID15 and ID31 where they carry out diffraction experiments using the poly-crystal structure as an atomic strain gauge. “ID31 is especially convenient to investigate the material close to the surface,” says Withers, “but then on ID11 and ID15 you have higher energies and we can study larger components.” Neutrons are a complementary tool in this research: they allow full-size engine assemblies due to their even higher penetrating power, although they provide less spatial resolution. In addition to the ESRF, the team also uses the Institut Laue-Langevin in Grenoble as well as the ISIS neutron source, and most recently Diamond (UK).

The benefits of this research go from underpinning the safety of the blades and their resistance to fretting fatigue and foreign object damage to extending the method to other applications: so far, the team has tested titanium alloys (normally used in fan blades and biomaterials too), but also stainless steel for applications in power plants. “In the case of aero engines, they are increasingly operating at higher temperatures and there is a continuous drive to make aircraft lighter. We need to find ways to make the materials and develop manufacturing processes that are up to the task and the ESRF helps us ensure that the science keeps up with technology,” says Withers.

M Capellas

References
A King et al. 2006 Mat. Sci. & Eng. 435–6
Focus on: industry and academia

The value of industrial research at the ESRF

The traditional gap between the communities of academia and the commercial world is narrowing and becoming less of a barrier as the two worlds increasingly seek to work together. Industry is rapidly realising the potential of research institutes and universities as vectors to help the development of technologies for applications in innovative commercial products.

In the last few years “open innovation”, where resources, ideas and know-how from both industry and academic research are combined to accelerate the innovation cycle, has become a path trodden increasingly by industry and academia to their mutual benefit.

The ESRF is no exception to this trend. Historically, the ESRF has been viewed by industry as difficult to access and not set up for its needs. However, we already run a small but significant programme of proprietary beam-time use by industry, particularly for protein crystallography in drug discovery by pharmaceutical and biotechnology companies. The ESRF also welcomes experiments from industry through its collaborations and partnerships with academia where proposals for peer-review beam time can be awarded as long as the results are published. Many peer-reviewed experiments carried out at the ESRF are associated with industry, either through a direct collaboration or by student or post-doctorate funding, but these links are often unknown to us and the potential for valuable and visible feedback to our funding bodies is lost.

One of our key objectives is for the ESRF to become more open and transparent for these academic–industrial experiments. In practical terms this means proactively supporting industrially associated work at the ESRF by including scientists and technologists from industry on the beam-time allocation panels that review proposals and by treating industrial applicants in the same way as academics. Of course, for this to work it also means that our users need to check the tick box on the beam-time application forms to let us know that industry is involved.

The ESRF is an exceptional tool financed by public funds, available to as broad a community as possible and our users’ experiments are far from all being about immediately applicable research. Fundamental research will remain as a pillar of the ESRF’s user experiments and indeed strengthened by industry becoming actively involved in experiments that open new horizons and lay the basis of future, innovative developments that industry can benefit from over a longer timescale.

In the longer term, opening the ESRF to industry and responding to its needs more visibly will better demonstrate the value of an international synchrotron centre of excellence that is able to help drive new developments directly having an impact upon the European economy. As industry starts to better appreciate the power of the ESRF’s X-ray beamlines – both our current and new facilities to be built as part of the Upgrade Programme – the proprietary programme with industry will be strengthened with opportunities for full service offers and R&D projects to solve the problems that industry brings to our expert scientists and facilities. The income that is generated through our proprietary work is used to support further staff and improve our beamlines to the benefit of all of our user communities.

In this issue of the ESRFnews, the “Focus on” section takes a detailed look at the innovative research that is being carried out at the ESRF, highlighting some of the successful stories of work with strong industry links, such as work with and from internationally recognised companies. These examples are just the tip of what we hope to see as a growing section of valuable research done at the ESRF.

S Pérez and H Reichert, directors of research

“One of our key objectives is to become more open.”
Boosting industrial users

“There are still companies out there who don’t know what the ESRF could do for them. There is a lot of potential – we just need industry to get to know us,” explains Ed Mitchell, business developer at the Industrial and Commercial Unit of the ESRF. The unit, founded in 2002, has attracted a steady number of industrial users to the ESRF until today. “We need to do more, though,” says Mitchell.

Today, this group is undergoing a makeover and it is adding more features to its services. On top of the data of experiments performed by companies, the service will now include full data analysis – “a complete service”. This will also include teaming up with specialists in the field from academia who can help to better answer the requests of the companies. “We need to come out of the cocoon where we have been until now and focus more on industrial users, without forgetting the academic sector,” says Mitchell. Academic users won’t be put on the side. On the contrary, they will benefit from the industrial work as well. This is the case, for example, of a catalysis reaction chamber built for and paid by Toyota. Today academic users can freely use it.

The ESRF will also team up with local partners to provide an optimal suite of facilities for industrial researchers. A project that is currently under preparation is the so-called “Technology Building”, set up by the Centre d’Energie Atomique, the ESRF and the Institut Laue-Langevin. This building would house tools for sample preparation for the ESRF and the ILL facilities, and complementary characterisation targeted for industrial users. If approved, it would have French funding and would be operational around 2013.

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Focus on: industry and academia

Tests at the ESRF aim to improve advanced high-strength steels

One of the main solutions to producing lighter cars lies in the selection of improved structural materials, such as advanced high-strength steels (AHSS). ArcelorMittal, a manufacturer of AHSS, in collaboration with the laboratory MATEIS (Institut National des Sciences Appliquées – INSA Lyon, France), carries out mechanical tests of this material at the ESRF to improve it.

The automobile industry has come a long way in terms of safety and its latest challenge is to provide environmentally friendly cars by reducing fuel consumption and CO2 emission. One measure that helps to achieve this is using advanced high-strength steels (AHSS) in their manufacture.

Car makers started using AHSS in the late 1990s in the so-called body-in-white structure of the cars. The main aim was to increase the material’s strength, giving the opportunity to make the cars lighter while keeping a high energy absorption during a crash. In comparison to the conventional high-strength steels (HSS) having yield strengths lower than 550 MPa, the AHSS exhibits yield strengths between 600 and 1500 MPa.

Dual-phase steels (DP) are the main metallurgical solutions for AHSS. The microstructure consists of hard martensite islands embedded in a soft ferritic matrix. Thanks to this bi-phase microstructure, the material has a good combination of strength and ductility. In order to go further it is now necessary to limit as much as possible the damage induced by deformation by microstructural design. The fraction of martensite used and its hardness play a major part in the damage nucleation but also in increasing the steel resistance. The task of researchers at ArcelorMittal is to find the right balance to avoid damage, while maintaining a high resistance. Caroline Landron, a PhD student funded by ArcelorMittal and based at INSA, explains that, when DP steels are forming, voids could appear in the structure. “We have to understand why and what are the impacts of the microstructure.”

The first step is to be able to characterise damage appearing when tensile tests are performed. For this, the team uses X-ray microtomography to picture the DP steels at the ESRF. “This is almost exclusively the technique that we use to track the void nucleation,” explains Eric Maire, director of research at INSA. The team has used ID15 and ID19, the first one being faster at scanning and the second one providing better resolution images. The researchers applied tensile tests to various DP steels (with different proportions of ferrite and martensite) on both beamlines and managed to quantify the damage. The results allowed the team to create and validate models of the nucleation and the growth of voids.

In the future, it could be desirable to carry out X-ray tomography on the material while it is being tested with even more realistic conditions than tension. “Once we have found the patterns on how the damage is made and where it takes place, we will try to design new microstructures that better resist damage,” explains Olivier Bouaziz, expert at ArcelorMittal.

M Capellas

Reference
C Landron et al. 2010 Scripta Materialia 63 973–976.
Optoelectronic devices consist of different semiconductor alloys lying on substrates. During the growth of the MQW laser-active region, different layers of semiconductors are sequentially deposited on the substrate, alternating well and barrier regions. In well regions, electrons and holes recombine to provide the laser light, while barrier regions are important for the electrons and holes confinement in the wells. The parameters that are able to modulate the laser wavelength needed to match the minimum adsorption of the optical fibres are the chemical composition and the width of both well and barrier regions.

For low-speed communications, the sequence of “0” and “1” containing the information is produced by directly modulating the MQW laser emission by a variable current. Such devices can be fully characterised using laboratory X-ray diffraction (XRD) and photoluminescence (PL) techniques. For high-speed communications, device instabilities prevent this simple solution and the MQW lasers are fed by a constant current that generates a constant emission, which is not carrying any information. To create the information, chips containing MQW lasers need to be modulated externally. This modulation is achieved with electroabsorption-modulator (EAM) devices, which are normally connected externally to the MQW laser. EAMs are also MQW heterostructures with an energy gap that can be modulated at high frequency applying an external potential (Stark effect). In such a way the EAM can switch from opaque to transparent for the light emitted by the MQW laser.

Scientists are trying to integrate both MQW laser and EAM, occupying a small area (typically 30 × 700 µm², so that in a single 2 inch InP substrate about 2 × 10⁴ devices may be potentially processed). The optimisation of these EML devices has, until now, been carried out by empirical approaches because of the impossibility to carry out a micron-resolved XRD study with laboratory sources. A team from the University of Turin (Italy), Avago Technologies and the ESRF has, for the first time, managed to directly measure the structure of these semiconductors thanks to the micrometre X-ray beam of ID22.

The selection of some of the 35 full XRD patterns collected moving from the MQW laser (SAG region) to the EAM (FIELD region) that allowed to obtain the fundamental structural parameters of the system.

The unprecedented characterisation gave the team the opportunity to determine the structure of the grown heterostructure with a monolayer resolution (3 Å) along the growth axis and with a micrometre resolution in the growth plane (i.e. to find out what has been empirically grown). This study, requiring a high flux of hard X-rays combined with a micrometre resolution can be achieved in very few beamlines worldwide, such as ID22.

“These results show us the way to improve the growth process, which was previously based only on a trial/error approach,” explains Carlo Lamberti, leader of the team and professor at the University of Turin.

M Capellas

References

In a technology-led world, optical-fibre communications allow, for example, people to be connected through the internet or cable-television signals. Multi-quantum well (MQW) electroabsorption-modulated lasers (EMLs) are semiconductors heterostructures used with this aim. An Italian team has managed to characterise it for the first time at the ESRF on the growth plane of both well and barrier parts of the heterostructure. The result is achieved by fitting the observed pattern using a model based on the dynamic theory of X-ray diffraction. Finally, the combination of synchrotron μ-XRD with laboratory μ-PL allowed the team to obtain the space-resolved chemical composition from the space-resolved lattice parameter.

Semiconductors play an extremely important role in communications technology.
An experimental antibiotic fights resistant bacteria

The structural biology beamlines at the ESRF have allowed scientists from GlaxoSmithKline (GSK) to visualise how a new type of antibiotic can kill bacteria that have proved resistant to other treatment.

The work was part-funded by the Wellcome Trust’s Seeding Drug Discovery initiative and the US Defense Threat Reduction Agency, a sign of the growing importance of public–private partnerships in antibacterial discovery.

It is estimated that in 2007 about 25 000 people in the EU died as a result of infections caused by multi-drug-resistant bacteria. Also, infections due to antibiotic-resistant bacteria resulted in approximately 2.5 million extra hospital days at a cost of more than €900 m (European Centre for Disease Control and Prevention, 2009).

Topoisomerase inhibitors, called quinolones, are commonly used antibiotics with reported worldwide annual sales of $7 bn in 2009 (B Hamad, 2010). Quinolones have been used as antibiotics since the 1960s, but bacteria are developing resistance. The GSK researchers have shown that a new class of “novel bacterial topoisomerase inhibitors” (NBTIs) work via a mechanism that is distinct from the quinolones (B D Bax, 2010). Both the new NBTIs and the well established quinolones target bacterial type IIA topoisomerases, trapping the enzyme in complexes with DNA, but they do this in different ways (B D Bax, 2010 and A Wohlkonig, 2010). Stopping this enzyme and trapping it in a complex with DNA is highly lethal to bacteria and prevents them from reproducing.

Using the structural biology beamlines at the ESRF, the scientists could see how the new experimental compound, called GSK299423, latched on to the enzyme topoisomerase in a different place to quinolones, enabling it to stop the same bacteria that are resistant to the older treatment (B D Bax, 2010). The new compound targets a binding site that has not previously been characterised structurally or exploited by available drugs, giving a structural basis for the action of a new class of antibacterial agents against a well validated drug target.

GSK299423 was approximately 70 times more potent against the topoisomerase enzyme from Staphylococcus aureus than another NBTI that progressed to human trials. “The structure was difficult to solve because the topoisomerase enzymes are inherently flexible, making it difficult to grow well ordered crystals. We had to make many different truncated forms of the enzyme, try many different DNA sequences and test hundreds of crystals in order to obtain a good high-resolution structure. However, when we had grown the ‘right crystal’, the high flux, low divergence and well collimated beams available at the ESRF made it relatively straightforward to collect a 2.1 Å dataset (on crystals that had a 93 × 93 × 410 Å cell, with one 170 kDa complex in the asymmetric unit),” explains Ben Bax, a member of the GSK team.

The new compound class is still at an early stage of drug development, and could become important for attacking antibiotic-resistant strains of bacteria, such as meticillin-resistant Staphylococcus aureus (MRSA), and against Gram-negative bacteria like Escherichia coli, Pseudomonas, Klebsiella and Acinetobacter. An added problem arises with Gram-negative bacteria, as they have an outer membrane surrounding the bacterial cell wall, which interferes with drug penetration. New medicines must not only be toxic to the pathogen, but must first overcome the entry barriers that stop the bacterial cell being reached.

M Capellas

References
The quest to reduce saturated fats

Saturated fatty acids in food increase blood cholesterol level, which has been identified as a risk factor for heart disease and stroke. The food industry is working on finding healthier alternatives to these fats, which are present in margarine or butter to give them firmness. Unilever scientists have visited the ESRF to investigate their most recent healthier substitutes.

The most common way to provide texture to oily food products is by having a network of small crystallites of triglycerides (also known as crystalline triglyceride hardstock) present, which is rich in saturated fatty acids. Saturated fat raises blood cholesterol and it is present, among others, in dairy products, chocolate, fatty meat and some prepared foods.

To find healthier alternatives to the crystalline triglyceride fat, scientists are looking for structurants that do not raise blood cholesterol. Researchers at Unilever discovered serendipitously that the mixture of $\gamma$-oryzanol with $\beta$-sitosterol could be used for this purpose. These materials belong to the class of plant sterol(ester)s that are actually known to reduce blood cholesterol, and $\beta$-sitosterol esters are added to some margarines, such as Flora pro·activ, for this specific purpose. In many aspects, the mixture behaves differently from a normal crystalline particle network and it is more reminiscent of so-called organogels, which raised questions concerning the supramolecular structures in these systems. “The ESRF covers all of the length scales involved in the structuring of this mixture, so our results encouraged us to pay a visit to the ESRF,” explains Ruud den Adel, research scientist at Unilever.

The team used small-angle and wide-angle X-ray scattering at the high-brilliance beamline ID2 and also carried out some complementary X-ray diffraction measurements at the Unilever labs. They found that the mixture of $\gamma$-oryzanol with $\beta$-sitosterol creates a network of tubules in edible oil (sunflower oil in this particular study) that form rapidly when cooled below the melting point of the gel. Potentially, tubule formation can be retained by controlling the water activity in the emulsion. “To exploit this effect in foods remains a challenge because product developers tend to have limited formulation freedom when designing a recipe,” explains den Adel.

M Capellas

References
ESRF improves vertical emittance and brilliance

As part of the Upgrade Programme, the Accelerator Division of the ESRF is increasing the brilliance and coherence of the photon beams from the undulator by the reduction of the vertical emittance to 5 pm.

Recently, the electronics of the 224 electron beam position monitors of the ESRF storage ring have been replaced by modern units making use of digital electronics (Libera electronics). A much improved resolution in the orbit measurement has been reached, which gives a number of benefits. For example, it is now possible to measure the lattice functions of the ring (beta functions) with higher accuracy. The higher precision combined with an improved algorithm of coupling correction has resulted in the operation of the ring in user service mode with a root mean square (rms) vertical emittance as small as 5 pm for several days in a row. This corresponds to a rms normalised emittance of 0.06 mm mrad. The emittance of the beam is permanently measured by different diagnostic tools located around the storage ring (two pinhole cameras combined with 11 beam-size monitors of bending magnet X-rays around 170 keV). The results are in good agreement with theory (A Franchi), which predicts some small variation of the apparent emittance along the ring circumference (the apparent emittance is defined by $\alpha^2/\beta$ where $\alpha$ is the rms source size and $\beta$ is the vertical beta function at the source).

With such a small vertical emittance, the vertical size of the electron beam inside an undulator is as low as 9 µm fwhm while the vertical divergence is 3 µrad fwhm. The coherence and brilliance of the photon beam has therefore reached the record values shown in figure 1. Experiments making use of the X-ray beam coherence, or needing a small X-ray spot size on the sample, will strongly benefit from such a beam on condition that the beamline optics are carefully designed to preserve emittance. Particular attention is needed on the reflective optics (rms slope errors) and on windows and filters to avoid the generation of small-angle scattering. Ultrahigh vacuum type beamlines (no windows) equipped with refractive lenses and zone plates should be able to make full use of this new small emittance photon beam. Reducing the vertical emittance from 30 to 5 pm has resulted in a reduction of the lifetime to 40 hours for 200 mA of stored current due to higher intra-bunch scattering between electrons (Touschek effect). This effect, however, may be remedied by increasing the number of injections per day or ultimately by operating in top-up mode.

To obtain such a low emittance value, the coupling between the horizontal and vertical betatron oscillation has been recorded and corrected by 32 skew quadrupoles located along the ring circumference. Nevertheless, some of the 72 undulator segments have a small residual spurious skew quadrupole field that varies with the magnetic gap and generates some apparent emittance, beyond the 5 pm level. As the gap of the 72 undulator segments is varied randomly (seen from the storage-ring control room), it results in a drift of the emittance, adding to the fluctuations due to thermal drifts. These emittance fluctuations are corrected in three steps: the full correction is updated periodically during machine studies, by minimising spurious resonance driving terms, and resulting in the smallest vertical emittance. Then the most perturbing insertion devices are equipped to further reduce the emittance.
with a feed-forward local correction using two dedicated skew quadrupoles at both ends of the ID straight section. Finally, the remaining perturbations are corrected by a periodic retuning of the nearest coupling resonance. Recent studies predict a further reduction of the vertical emittance by increasing the number of available skew quadrupoles along the ring circumference (A Franchi).

Finally, as shown in figure 1, a higher brilliance exceeding the $2 \times 10^{21}$ range is within reach: longer straight sections (6 m and 7 m) are being implemented as part of the Upgrade Programme, allowing an increase in length of in-vacuum undulators up to 5 m, and the ESRF can be steadily operated at 300 mA as demonstrated in a number of machine-dedicated tests in 2010. A further improvement could also be achieved by equipping a long straight section with cryogenic undulators. Although a further reduction of the vertical emittance by a factor of 2.5, by means of additional skew quadrupole correctors, can be implemented at a low cost, the increase of the ring current has financial consequences of a far greater range and is therefore under debate.

L Farvacque and P Elleaume on behalf of the Accelerator and Source Division

Reference
A Franchi et al. to be published.

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**Figure 1:** Solid curve: brilliance of X-rays from the two in-vacuum undulators installed on ID27 for high-pressure studies. Each undulator segment has a period of 23 mm, a length of 2 m and is operated with a minimum gap of 6 mm. Dashed curve: as above but with 300 mA stored beam (routinely reached in machine dedicated time) and two 2.5 m in-vacuum undulators as foreseen within the ESRF Upgrade Programme.

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In radiotherapy and chemotherapy for cancer treatment there is a delicate balance between attacking and killing the cancer cells and minimising harm to non-cancerous tissues.

To minimise or even eliminate this “collateral” damage and make the most of the therapeutical effects, scientists have been developing nanoparticle complexes that can go directly to the cell nucleus and amplify the healing effects by targeting the cancer cells.

A multidisciplinary European collaboration led by researchers from the University of Birmingham (UK) has succeeded in the development of a technique that allows the detection, with pinpoint accuracy, of clusters of nanoparticles inside a cell.

These nanoscale particles, which can carry and deliver imaging agents and therapeutic drugs, could become an exciting new strategy for diagnosing and treating diseases, such as cancer.

“Just a few nanoparticles delivered precisely to where needed could be sufficient to achieve a patient’s treatment. Visualising where exactly the nanovectors go and in what number is extremely important,” says Boris Kysela of the University of Birmingham and co-principal investigator on the study.

A research team comprising bioscientists and chemists from Birmingham and physicists at the ESRF and Institut National de la Santé et de la Recherche Médicale (INSERM) in Grenoble (France) probed the cellular uptake of nanoparticles using the unique nanoimaging facility at the ESRF, ID22NI.

“The technique of X-ray fluorescence microscopy at the ESRF is an invaluable tool that helps us to test which of our designs are the most efficient, with incredible sensitivity, speed and spatial resolution,” explains Zoe Pikramenou, co-principal researcher. It allows detection of a handful of particles inside the cell and pinpointing of their position within the cell with remarkable accuracy. This is crucial for studying their action at the low-dose levels that might be used in patients.

“Five days of work at the ESRF can be the equivalent of several months of effort using other, less efficient, techniques.”

The research team demonstrated that gold and platinum nanoparticles coated with light-emitting agents can reach the cell nucleus and be imaged with unprecedented sensitivity. “I didn’t expect it to work out so quickly,” says Kysela. “The X-ray fluorescence imaging also helps enormously with analysing possible long-term genotoxicity issues, which is often an overlooked aspect in nanomedicine developments,” he adds.

In cancer treatment specifically there is a delicate balance between attacking and killing the cancer cells and minimising harm to non-cancerous tissues. To minimise or even eliminate this “collateral” damage the next generation of nanodevices is already being tested that can actively seek tumour cells and amplify the healing effects by targeting the cell’s genetic material – DNA.

“The team’s aim now is to drive the concept forward.”

M Capellas

Reference
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E Pebay-Peyroula: juggling many roles

Eva Pebay-Peyroula, who is director of the Institut de Biologie Structurale (IBS) among other positions, has had a close relationship with the ESRF for many years.

With a gentle and mild-mannered demeanour, at first glance Eva Pebay-Peyroula does not come across as the high-flyer that she really is. At 54, this physicist turned structural biologist leads the IBS, holds a professorship at the University Joseph Fourier in Grenoble and is a member of the French Académie des Sciences. The latest accolade of this French–Austrian scientist is the presidency of the Agence Nationale de la Recherche (ANR), the organisation that decides how to distribute funding to different scientific projects nationally, which she has held since June.

To people outside of France, all of these roles might not mean much, but the way that she got the ANR job highlights the high level of these positions: “I was already a member of the ANR steering committee, but the presidency of it was unexpected. One day, out of the blue, I got a call from Valérie Pécresse, minister for higher education and research, on my mobile phone asking me if I wanted the job. I don’t know how she got my number, but it was quite a surprise,” admits Pebay-Peyroula.

Despite her long and prosperous career, when asked about one of the most exciting work-related moments, the ESRF comes into the picture: “I think that one of the best times was when, as a user at the ESRF, we first achieved good diffraction from crystals on ID13 after working hard for a long time to get optimal crystals. This was back in 1995 and 10 minutes after this milestone the director of research at the time, Carl-Ivar Brändén, was already on the beamline,” remembers Pebay-Peyroula. This achievement was possible thanks to a crystallisation method created by collaborators of Pebay-Peyroula at the University of Basel (Switzerland) and to ID13, the first microfocus beamline. It was even more of a feat because “no-one believed in the project until it actually worked”, she says. The results were published in Science in 1997 in the paper “X-ray structure of bacteriorhodopsin at 2.5 angstroms from microcrystals grown in lipidic cubic phases”.

The ESRF is, therefore, one of the tools that she uses in her research on membrane proteins, which is still very close to her heart. “I try to go to the experiments as much as I can. I think that it is important to be in touch with science,” she says. “This tool is essential in the study of the structure and function of membrane proteins,” she acknowledges.

Although today she is more of an administrator, she still dedicates time to her own research. She combines this with her teaching duties at the University (one-third of a full-time teaching load, “which is ideal”). She has played an important role in the set-up of the Partnership for Structural Biology, with the IBS being one of the members. “There is still a long way to go because people from the IBS don’t meet so often with the other three partners. However, the moving of the IBS buildings to the ESRF-ILL-EMBL site in the near future will certainly bring people closer, so I am not worried.”

Gender obstacles

It might sound like a stereotype, but science is still largely dominated by men. So how does a woman get into this world and succeed? Pebay-Peyroula suggests that she’s always been very focused, although no-one ever “pushed” her to have a career. When she began her PhD she also started a family. Between her PhD and post-doctoral position she had three children and managed to stay in tune with science. “It is important not to wait too long to have kids as you can always come back to science,” she says. Later, when she had been at the IBS for some years, she would prefer the night shift: “At night the children didn’t need me, and I could finish at 7.00 a.m., go home and take them to school.”

She has found, however, several obstacles throughout her career. It was not straightforward for her to get a research group when she arrived at the IBS, even though she had the support of the director at the time. Changing the culture of a masculine environment took a while, but today 50% of the staff at the IBS are female.

With such a career, she’s done it all, or almost. “I don’t have many other ambitions. I am happy to be where I am,” she confesses. “More evolution in my career would probably force me to move to Paris, and I really don’t want that. I like the mountains too much and, despite the very long hours spent at work, I still try to go hiking with my husband at least once a week.”

M Capellas
In the corridors

**Goodbye Walkman**

Some months ago it was the floppy disk, now it’s time for the Walkman to disappear. Sony has announced that it stopped its production last April. Launched in Japan on 1 July 1979, Sony has, during these 31 years, sold more than 220 million units worldwide.

**Google celebrates X-rays anniversary**

The internet search engine Google has celebrated the 115th anniversary of the discovery of the X-ray by Wilhelm Röntgen. Google posted a doodle (the image on its homepage) on the subject on 8 November. In it, the logo of Google appeared as if it had an X-ray scan, with bones forming the letters along with several other items, such as keys, coins and a rubber duck.

Röntgen’s work with X-rays, which started by chance, led him to receive the Nobel Prize in Physics in 1901 “in recognition of the extraordinary services that he has rendered by the discovery of the remarkable rays subsequently named after him”.

Other scientific achievements that have been honoured by the Google doodles are the 20th anniversary of the Hubble telescope and the birthdays of Isaac Newton, Albert Einstein and Leonardo da Vinci.

**Flower has largest known genome**

A flower called *Paris japonica*, originally from Japan, has just broken the world record for the largest known genome. Its genome contains 150 billion letters, 15% more than the previous holder, the marbled lungfish. In the publication, the authors explain that there are biological consequences associated with increasing DNA amounts, such as reduced brain complexity in some animals and increased risk of extinction in plants.

**Reference**

The insertion device group contributes in maintaining the accelerator at the forefront.

The insertion device group has existed since the early days of the ESRF. In fact, it was one of the key groups of the facility, which was going to be one of the first synchrotron sources functioning with many insertion devices (ID). “The ESRF is the first large source where the need for IDs was significant,” explains Joel Chavanne, head of the group.

An impressive figure of 130 undulators and wigglers endorses the work of this group, which is made up of four engineers and four technicians. Their goal is to design and procure parts of the IDs, define their magnetic system and field correction, and to install and maintain the IDs, including software control. The team produces between five and 10 IDs every year, though the number of IDs installed varies from year to year. The ID group is recognised worldwide in many aspects. For example, the 3D magnetic field simulation software RADIA, developed at the ESRF, is presently used in almost all facilities for magnet design. Similarly the ESRF field measurement techniques or field correction methods have been adopted in several other facilities (SOLEIL, DIAMOND, ALBA and SLS). On the basis of these successful developments, technology-transfer agreements on IDs have been set-up between the ESRF and two European companies (Danfysik in Denmark and Bruker in Germany) for several years.

The Upgrade Programme of the ESRF is already taking its first steps and the ID group has been very involved with this for two years (they have already received magnetic assemblies for 11 IDs). The team has also improved the design of in-vacuum undulators, they will be 2.5 m long – a first version is already under construction and will be used in UBL4. There are a few additional tasks that come on top of the usual ID group work, such as dealing with the field-measurement magnets that are due to be used in the accelerator, as well as developing specific magnetic systems in canted straight sections.

M Capellas

Movers and shakers

NWO Spinoza Prize
Piet Gros

Piet Gros, a user on the structural biology beamlines at the ESRF and professor of molecular crystallography at Utrecht University (the Netherlands), has been awarded the Netherlands’ highest distinction in scientific research – the NWO Spinoza Prize. Gros received this prestigious award and a monetary sum of €2.5 m to devote to his research in recognition of his pioneering contributions to unlocking the three-dimensional structure of the complement component 3 (C3) protein. This very large protein is part of the immune system’s oldest branch, which is still present in humans. The defensive mechanism of this part of the immune system, which attacks all cells, including the body’s own, has the potential to cause havoc in the body. The ESRFnews dedicated an article to his work in the December 2008 issue, pp 12–13.

CNRS Gold Medal
Gérard Férey

France’s highest distinction in scientific research, the CNRS Gold medal, has been awarded in 2010 to the chemist and ESRF user Gérard Férey, professor emeritus at the Université de Versailles Saint-Quentin-en-Yvelines near Paris (France). This prestigious annual prize rewards the works of a prominent personality who has made an exceptional contribution to the dynamism, reputation and influence of French scientific research.

Férey is a researcher in the physicochemistry of solids and inorganic or hybrid materials. He specialises in the design of hybrid porous materials, in particular for the storage of CO₂ or medicines. With the help of his team, he predicts and explains the behaviour of these nanomaterials, which have a wide range of useful properties and potential applications in the fields of energy, sustainable development and healthcare. The beamlines that Férey has used the most are ID31 and the Swiss–Norwegian beamline BM1.

Director of administration
Manuel Rodriguez Castellano

The ESRF has had a new director of administration, Manuel Rodriguez Castellano, since 1 October and he will hold this position for the next five years. He has acted as temporary director of administration since April. Rodriguez Castellano, a lawyer, who holds a masters in business administration, arrived at the ESRF in 1990. He has a broad knowledge of the ins and outs of the facility, as his latest position was as secretary of the council and adviser of the director-general of the ESRF. He also founded and led the industrial and commercial unit at the ESRF since 2002 until now. Previously, he had been working in the administration division as head of the central services first, and later as head of the commercial and central services. Before arriving at the ESRF, he worked for more than three years at the European Commission, in the former DG XIII, specialising in legal matters and human resources. He was also associated to the management of large European scientific programmes. His first professional experience was at the Spanish Embassy in France.
Karlsruhe Institute of Technology (KIT) is the result of the merger of the University of Karlsruhe and the Research Center Karlsruhe. It is a unique institution in Germany, which combines the mission of a university with that of a large-scale research center of the Helmholtz Association. With 8000 employees and an annual budget of EUR 650 millions, KIT is one of the largest research and education institutions worldwide.

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**Your profile:** A graduate degree (master or diploma) in physics, mathematics, engineering or computer science, solid knowledge of electrodynamics is expected, programming skills are required and knowledge of magnet design is favourable, strong interest in accelerator physics, a high motivation and the ability to work independently, willingness to travel and to present results of the work at international conferences.

This work package will be distributed between the positions in accord with the candidates. The positions are limited to three years (two years plus one year extension). The salary grade is TV-L E 13.

KIT is pursuing a gender equality policy. Women are therefore particularly encouraged to apply. If qualified, handicapped applicants will be preferred.

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The Paul Scherrer Institute is with 1400 employees the largest research centre for the natural and engineering sciences in Switzerland and a worldwide leading user laboratory. Its research activities are concentrated on the main topics structure of matter, energy and environmental research as well as human health. The Swiss Light Source (SLS) is one of the most advanced synchrotron radiation sources worldwide. The Research Department for Synchrotron Radiation operates several state-of-the-art undulator beam lines in the hard X-ray domain. It conducts an intense in-house research as well as instrumentation program with special emphasis on detectors, imaging techniques and on-line beam diagnostics. The Accelerator Concepts Section of the Large Research Facilities Division at PSI supports the development of new accelerators and the consolidation and improvement of existing machines, contributing to the fields of theoretical beam dynamics, studies and simulations, accelerator design, accelerator commissioning and development of simulation tools and applications. The opening for postdoctoral fellow is a joint position between the two divisions. We are looking for a

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You are responsible for the development of an extension of the fast global electron beam orbit feedback system, with the aim to stabilize the X-ray beam in position and angle at the position of the sample over a wide frequency range. To this end you will characterize the dynamic response properties of the electron beam and X-ray beam position monitors. Based on these results, beam dynamics studies will be carried out to determine the influence of the envisaged feedback system extension on the global orbit stability. The system will require a completely transparent X-ray optical system. Automatic initialization, self calibration and analytical modeling of the beam-transport by means of geometrical optics is hence a prerequisite. Feedback interlocks will be necessary in order to minimize the risk of accidental orbit distortions or even beam dumps due to the system. Since your contribution is most critical for the operation of the SLS you will have to design, implement and test the feedback system extension in close collaboration with the responsible beam dynamics and diagnostic experts as well as the corresponding beam line scientists.

**Your profile**

You hold a PhD degree in physics, with experience in theoretical and experimental accelerator physics in the fields of beam optics or in the field of X-ray optics. You are a skilled user of common related software tools (e.g. MAD, Elegant, MATLAB, XOP, SRW) and a programming language, ideally C/C++. You have basic knowledge of electronics and related measurement techniques. Experience in simulation of X-ray beam lines is advantageous. You enjoy the work in an interdisciplinary and multi-national research team. You are motivated to expand your knowledge and experience and look forward to the development of novel feedback systems exploiting synergies between the accelerator and the beam line domain. Good communication skills in English are expected, knowledge of German is advantageous.

For further information please contact: Dr Michael Boege, phone +41 56 310 45 88, michael.boege@psi.ch or Dr Meitian Wang, phone +41 56 310 41 75, meitian.wang@psi.ch.

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<td>± 1/± 5</td>
<td>EP3C16</td>
<td>Single Ended</td>
<td>65 MS/s</td>
<td>30</td>
<td>12</td>
<td>0.19/1.5</td>
<td>64 ch</td>
<td>32 ch</td>
<td>32 ch</td>
<td>-</td>
</tr>
<tr>
<td>751</td>
<td>± 0.5</td>
<td>EP3C16</td>
<td>Single Ended Differential</td>
<td>1-2 GS/s</td>
<td>500</td>
<td>10</td>
<td>1.8-3.6/14.4-28.8</td>
<td>8-4 ch</td>
<td>4-2 ch</td>
<td>4-2 ch</td>
<td>-</td>
</tr>
<tr>
<td>761</td>
<td>± 0.5</td>
<td>EP3C16</td>
<td>Single Ended Differential</td>
<td>4 GS/s</td>
<td>Lbd</td>
<td>10</td>
<td>7.2/57.6</td>
<td>2 ch</td>
<td>1 ch</td>
<td>1 ch</td>
<td>-</td>
</tr>
<tr>
<td>742(2)</td>
<td>± 0.5</td>
<td>EP3C16</td>
<td>Single Ended</td>
<td>5 GS/s</td>
<td>Lbd</td>
<td>12</td>
<td>0.128</td>
<td>32+2 ch</td>
<td>16+1 ch</td>
<td>16+1 ch</td>
<td>-</td>
</tr>
</tbody>
</table>

(1) AMC: ADC & Memory controller FPGA, ALTERA models available: EP1C4: Cyclone (4,000 LEs), EP1C20: Cyclone (20,000 LEs), EP3C16: Cyclone III (16,000 LEs). (2) Switched capacitor.