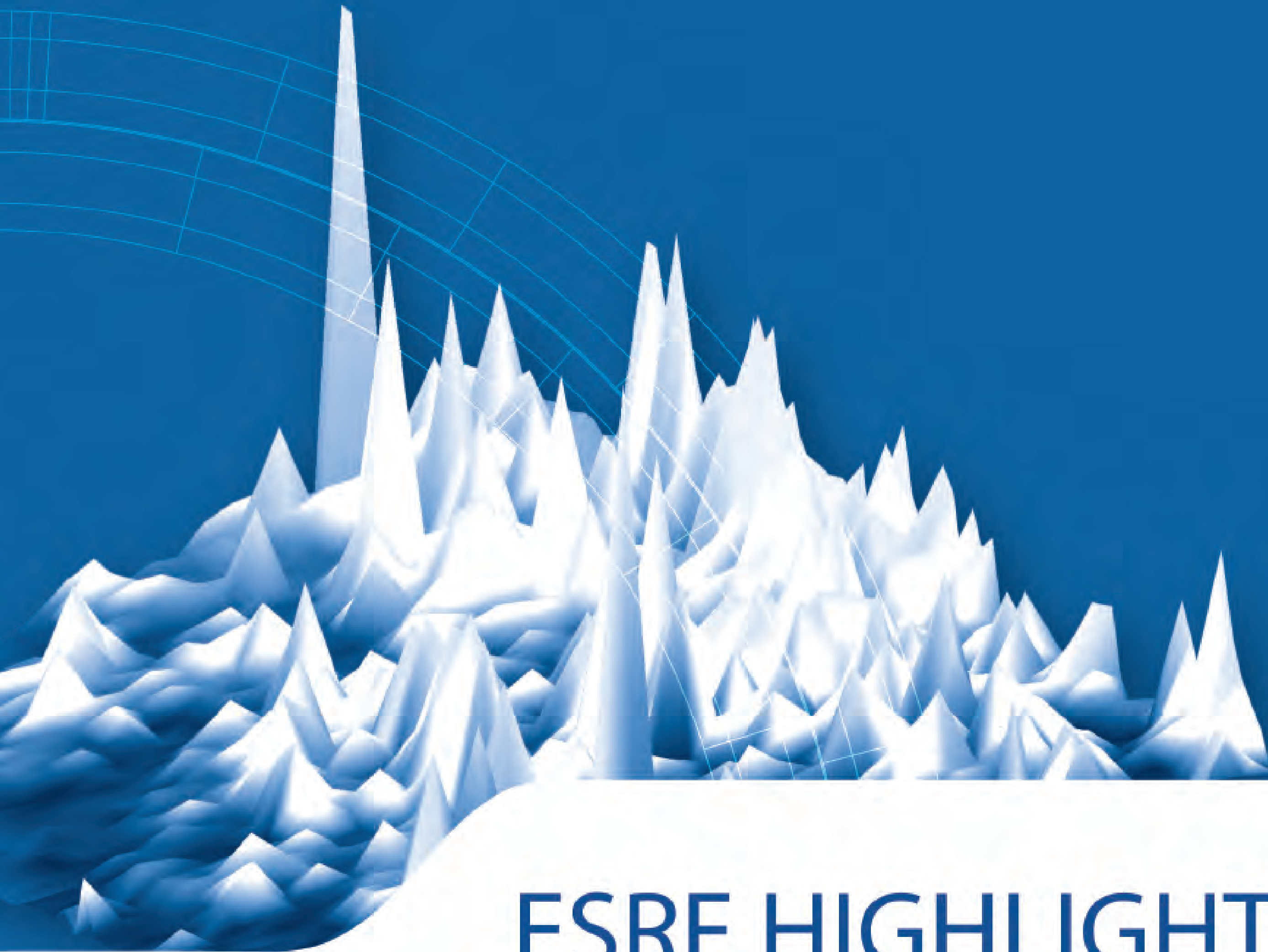
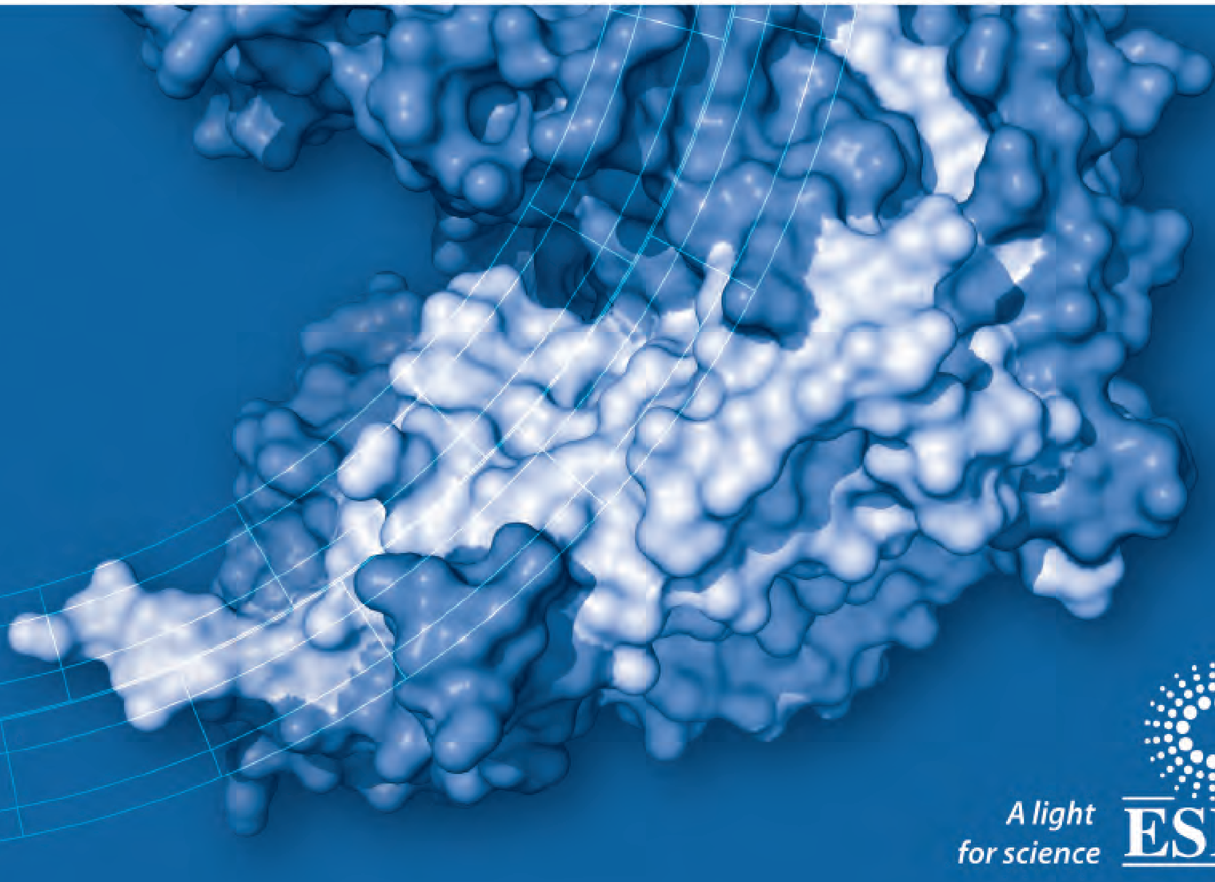


ESRF HIGHLIGHTS
2010



A light
for science

ESRF

Auszug aus:
(Extraktion from:)

HIGHLIGHTS 2010

ESRF
European Synchrotron Radiation Facility

Dear Reader

Credit: ESRF / Molyneux Associates.

The operation of the ESRF in 2010 has been as excellent as in previous years, characterised by outstanding scientific productivity and by record-breaking performance of the accelerator complex.

The number of proposals, experimental sessions, user visits and publications in peer-reviewed journals was again very high, comparable to the record figures of 2009. Details are outlined in the chapter on *Facts and Figures*.
The scientific highlights in the following chapters confirm the important trend of coupling increasingly smaller X-ray beams with X-ray techniques such as scattering, diffraction and spectroscopy. They also underscore an increasing use of coherence in many experiments and in different disciplines, both in the traditional fields of materials science, condensed matter physics, chemistry and life sciences, and in the emerging fields of palaeontology, environment and cultural heritage.

In parallel to the user operation, the Upgrade Programme is now in full swing with important progress in all areas:

1) Outstanding results have been achieved in the Source Upgrade: 6 m straight sections were installed for several beamlines; operation at 300 mA was successfully demonstrated; and good progress was made in the refurbishment of the RF system, notably for the new solid state amplifiers.
A special effort was devoted to the stability of the source which made it possible to reduce the vertical emittance to a world record value of less than 5 pm in User Service Mode. The increased brightness benefits notably the micro- and nano-beams.
The High Pressure Beamline ID27, for example, now serves its users with a world record brightness of almost $1x10^{21}$ photons/s/mm^2/mr^2/0.1bw in the 200 mA operation mode.

2) The evolution of the beamline portfolio has been progressing well, despite the new challenges due to the need to reduce the number of public beamlines. The eight Upgrade Beamlines (UPBLs) are being constructed as planned and the major beamline refurbishments linked to the UPBL construction should remain unaffected. UPBL10 (MASSIF) and UPBL11 (TEXAS) are already under construction, and UPBL4 (NINA), UPBL6 (Inelastic Scattering) and UPBL7 (Soft X-rays) have entered into the construction planning phase. Most other UPBLs have had their Technical Design Report (TDR) presented to and supported by the Science Advisory Committee (SAC), which in turn is kept constantly abreast on the evolution of the beamline portfolio.

3) The instrumentation development programme recorded important achievements: these include delivery in user mode of nano-beams down to ~60 nm using both K-B and compound-refractive-lenses; precision mechanics for nano-optics; commissioning of a Pilatus-6M 2D pixel detector on a Structural Biology beamline; commissioning of the liquid phase epitaxial deposition apparatus to prepare unique scintillation materials for hard X-ray detection in imaging experiments; and development of unique, powerful software packages for instrument control and on-line data analysis.

4) The Experimental Hall extension project (EX2) is ready for tendering with a reduced scope imposed by budget constraints. The new data centre in the Central Building to keep up with the increasing computing needs is nearing completion and will enter service in 2011.

2010 will be remembered as the year when important changes began, and new opportunities arose for the ESRF. The economic situation in Europe requires the ESRF to evolve: certain member countries, despite continued support to the ESRF, cannot finance our budget for some years to come at the levels originally foreseen. ESRF Management and Council have worked hand in hand on a scheme to alleviate these financial difficulties. On 30 November, Council unanimously adopted a resolution allowing two member countries to reduce their financial contributions for three years, and this without compromising the quality of the scientific programme.
All twelve member countries and seven scientific associates have renewed their long-term commitment to the ESRF, and especially to the continuation of its intergovernmental convention.

The resolution leads to a 6% budget reduction during 2011-2013 which shall be absorbed without compromising the quality of service for the 4000 scientists who use the ESRF. However, a reduction of this size meant difficult decisions had to be taken in 2010, and more lie ahead in 2011: the number of beamlines, and the operation time of the accelerator complex, must be reduced and some deliverables of the Upgrade Programme revised. These reductions shall be implemented in a way to limit as much as possible the impact on the scientific community. This impact will, however, to a large extent address users from countries forced to reduce their financial contribution, and which in return accepted a limitation of their beamtime.

The years ahead will be challenging for synchrotron science in general. Spectacular efforts over the past ten years saw the construction of excellent new synchrotron sources in particular in Europe, which reinforced its long-standing leadership. Today, important investments are foreseen in the U.S. and in Japan. More importantly, a strong programme is developing in Russia – building on a long tradition in synchrotron science – and in emerging market economies such as Brazil, China and India where strong scientific communities already use synchrotrons all over the world.

In the face of reduced resources in Europe, maintaining the present frontline position will need careful coordination to emphasise the complementarity of the ESRF with the other synchrotron sources. This will address issues like cost containment, efficiency, excellence in user services, technical developments and governance. Without coordination across Europe, we cannot maintain our leadership nor will we succeed in opening our laboratories to innovation, industry and new communities.

I am convinced that the ESRF, working in concert with others, can maintain a world leading role. We will create new opportunities for more unique beamlines on free insertion device straight sections of the ESRF storage ring. I expect new partners to be interested in exploiting these new and unique possibilities. The Council Resolution invites Management to attract, over the next three years, new members and scientific associates and to investigate other possible ways of collaboration with third parties. In parallel, Council and Management will work on new schemes where the funding of ESRF's needs is more closely linked with the use by scientists from the different members countries.

The first phase of the Upgrade Programme, despite the reduced building construction programme and a slightly lowered investment capacity for the other projects, maintains all innovative features enabling the ESRF to stay attractive to its users in the long term. These include eight unique Upgrade Beamlines for delivery by 2015. In parallel, Management has started reflecting on the second phase of the Upgrade Programme. A revised plan, along with options taking into account the new financial context will be presented to Council in spring 2011 with the aim to start discussions on new UPBLs with SAC and the User Communities in 2012, possibly beginning with the Users Meeting in February of that year.

In 2011, the Upgrade Programme will have a very limited impact on user operation, despite the start of construction work for EX2 in September 2011. Beamtime delivery should not be reduced by more than two weeks. In 2012, however, a long shutdown is planned with significant reduction of user operation from December 2011 to April 2012, and in August and September 2012. The overall reduction of beam delivery in 2012 will be about four months, with a return to normal user operation in 2013.

There have been some successful developments for new partnerships. In June 2010, the ESRF and the ILL launched the Partnership for Soft Condensed Matter (PSCM) which is now developing a programme to attract further partners from academia and industry. Partnerships and collaboration ideas are also developing in extreme conditions science, palaeontology, metallurgy, and technologies for synchrotron and neutron science. The two existing and future partnerships will greatly benefit from the new Science Building, located between the ESRF and the ILL with a direct connection to both facilities for the benefit of all users. This building, funded by French regional and local authorities, will be commissioned in 2012.

I would like to thank our Member and Associate Countries, and in particular their delegates to Council, AFC and SAC, for their continued support and trust. In particular, I wish to thank the Chairman and the Delegates of Council for having developed with Management a pragmatic solution to a difficult funding problem. Thanks to these efforts, the excellence of the ESRF will be maintained and new opportunities have been created. I am also very grateful to the members of the beamtime allocation panels and of the beamline review committees for their hard work assuring the scientific life of the facility. Special thanks go also to the European Commission which in 2008-2010 has provided crucial support through the ESRFUP contract for the preparation of the ESRF Upgrade. Today, through further opportunities given to the projects on the ESFRI roadmap, it continues supporting the ESRF in a very visible way. Special thanks go also to the French authorities, in particular the *Ville de Grenoble*, the *Grenoble-Alpes Métropole*, the *Conseil Général de l'Isère* and the *Région Rhône-Alpes* for granting the ESRF and the ILL funds for important infrastructure projects like the new Science Building and a new site entrance which enormously enhance our scientific visibility.

In this issue of the Highlights, a special thanks goes to all ESRF staff who have demonstrated a formidable motivation, hard work and perseverance in providing support to our users and in developing the Upgrade. Last but certainly not least, I wish to thank the thousands of excellent and dedicated users who make outstanding science possible, a few examples of which are outlined on the following pages. With their wonderful science carried out at the ESRF, they make all our efforts more than worthwhile.

Francesco Sette,
ESRF Director General.

Status of the Upgrade Programme

Progress during 2010

2010 saw the start of major works for the execution of Phase I of the Upgrade Programme with the first new beamlines now under construction in the existing experimental hall. Up to this point, works within the Upgrade had only minor impact on user operation, performance and productivity of the ESRF. A proposal for a new scheme to allocate public beamtime at the ESRF has been endorsed by SAC and Council and is now entering its implementation phase.

New Buildings

The project for the extension of the experimental hall is in the preparatory phase for the building works tenders. The preliminary design report was officially approved in May 2010 and the detailed design report in November 2010. These detailed studies have allowed the project to reach maturity. Adjustments to the initial Building Programme, including the extension of ID16 (**Figure 1**), have been made in order to meet both the scientific and budgetary requirements.

Credit: Sud Architectes.

Fig. 1: Architects view of the future ID16 building housing the two stations of the NanoImaging/NanoAnalysis (UPBL4 - NINA) project.

Progress in the studies allows technical solutions to be considered for the most challenging issues of the project. The construction schedule is already well defined and has been fixed in a way to minimise the impact on the user operation. The building works are planned to start in September 2011. The timescale includes two long shutdowns of the facility. The first shutdown (from December 2011 to April 2012) will be dedicated to the demolition of existing structures, modifications of existing networks and creation of the foundations for the extensions. The second one (a few weeks during the normal summer shutdown in 2012) will be dedicated to the completion of the 4 000 m^2 of high quality concrete slab on which many of the new beamlines will be constructed.

In parallel, and within the frame of the State/Region contract (CPER), studies are progressing for the construction of the Science Building (under the authority of the ILL), the extension of the restaurant and a new site entrance on the Avenue des Martyrs (under the authority of the ESRF). The CPER programme will enhance the scientific life and increase visibility of the EPN science campus.

Preparatory works have been started to free the space for the construction of the IBS2 building by moving the works committee to the centre of the ring and the subcontractor premises next to the technical buildings close to the river Drac. The IBS2 construction will start in May 2011 with a delivery planned for the beginning of 2013.

Upgrade of the Source

Upgrade of the accelerator system is progressing well. The much improved orbit measurement, resulting from the installation of the new electronics driving the electron beam position monitors, has enabled a higher precision in the horizontal to vertical coupling correction. The emittance of the electron beam has been reduced and stabilised below 5 pm for periods of up to a full week. An improved orbit stabilisation system is under development; it was made possible thanks to the new digital electronics.

The transformation of the straight sections of ID18 and ID30 for the accommodation of 6 m long undulators has been completed. New magnets, vacuum chambers, and undulators are under manufacture. An ambitious RF upgrade programme is being preparated that includes the replacement of some high power klystrons by solid state amplifiers and the development of new cavities with higher order modes damping. In 2010, the storage ring has been routinely operated with 300 mA of current during Machine Physics runs. The accelerator upgrade work was carried out during planned shutdowns and had no detrimental consequences on the User programme.

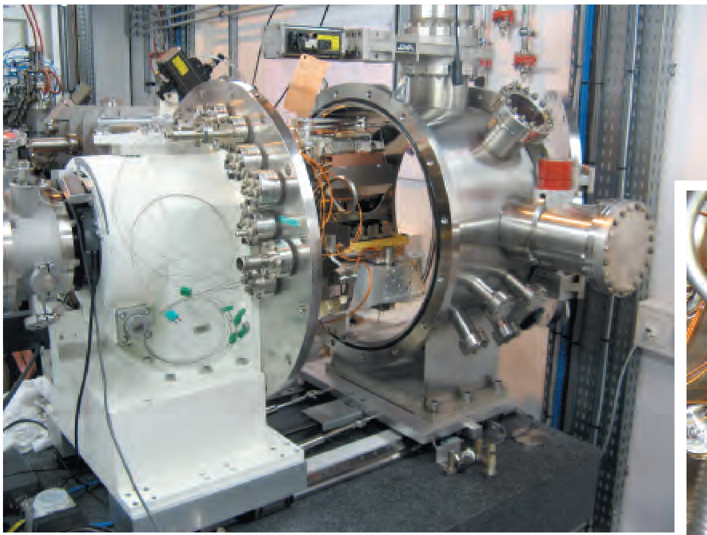
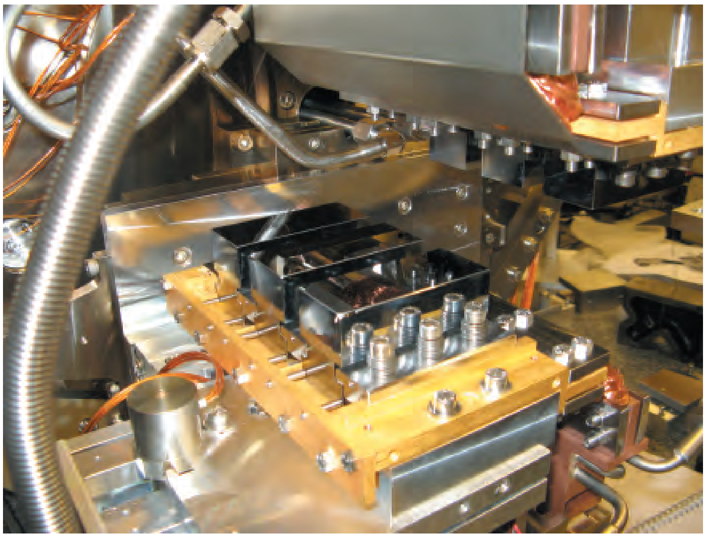


Fig. 2: The EXAFS beamline BM23 is the first new beamline to commence user operation following an upgrade with transfer from BM29. Left: Monochromator showing translation stage to change pairs of crystals; Below: Close-up of the 3 pairs of crystals (111, 311, 511), which enlarge the accessible energy range.



Renewal of Beamlines

Budgetary constraints have been absorbed mostly by further refining the number of beamlines to be moved in the floor plan for the public beamline portfolio of the ESRF while preserving the number of Upgrade Beamline (UPBL) projects at eight. The revised floor plan reduces the number of moving beamlines by three with the additional benefit of avoiding lengthy shutdown periods of the respective beamlines for users. The new floor plan has been endorsed in 2010 by SAC and Council for implementation.

Conceptual Design Reports (CDRs) and Technical Design Reports (TDRs) for five UPBL projects defining ten independent experimental stations have been produced, externally reviewed, and approved for execution in 2010. Work on CDRs and TDRs for the sixth UPBL and extensive refurbishment of the ID10 complex as well as ID19 has been started in parallel. The first new beamline, BM23, has finished its constructions phase and will commence full user service with the start of the 2011/I run, to be followed by UPBL11 finishing its construction phase in 2011 (Figure 2). Upgrade of instrumentation has already been started on all eight UPBL projects (Figure 3).

Fig. 3: T. Schulli and G. Carbone, scientists at beamline ID01 (UPBL1), with their new diffractometer for nanodiffraction analysis.

Enabling Technologies and Instrumentation

The Instrumentation Services and Development Division (ISDD) is deeply involved in the implementation of the Upgrade Programme for both the Experiments Division (ExpD) and Accelerator and Source Division (ASD).

Driven by the first UPBL projects, several key technological areas have been identified, *e.g.* X-ray mirror engineering, diamond technologies, nanofocussing optics, online data analysis, high-rate data collection. Expert working groups have been created to find innovative and reliable solutions. When possible these solutions are generic to allow cost-effective adaptation to multiple beamline projects. All ISDD scientists and engineers provide expertise in the preparation of TDRs ranging from ray-tracing simulation and heat load modelling to producing cost estimates for entire instruments.

Although the X-ray detector programme is still in a re-definition stage, several key elements of this programme have been started, including the implementation of a liquid phase epitaxy laboratory to secure the procurement of high quality scintillators. A collaboration contract with Science and Technology Facilities Council (STFC) for the production of a Ge microstrip detector for UPBL11 has been signed, as well as a three-year collaboration contract with PSI for the development of the EIGER detector. A new framework for imaging detectors, LiMA - Library for IMage Acquisition, has been developed. LiMA offers standardised interfaces with enhanced capabilities that are being developed in collaboration with other synchrotron facilities to ensure compatibility with a wide range of 2D detectors. Development of GPU accelerated data processing was successfully implemented for tomography reconstruction and will be adapted for other scientific applications. Concerning the beamline control electronics, more than 1000 motors are being controlled with standardised IcePAP electronics on beamlines. The UPBLs will also be equipped with these controllers.

Several critical X-ray optics projects such as high reflectivity X-ray multilayers, sub-60 nm KB mirrors, diamond monochromators and beam splitters and compound refractive lenses (CRLs) have been developed. The ESRF established a long-standing programme with several companies and academic institutes to ensure the production and tailoring of high-quality diamond single crystals for various applications. A new concept of transfocators combining linear and 2D CRLs was developed and installed at ID06. New beryllium linear refractive lenses were tested under white beam illumination at ID06. This heat-load test confirmed high stability of the lenses opening the opportunity to use new in-vacuum and white beam 1D transfocators for the ESRF upgrade beamline projects (*e.g.* UPBL4). Finally, in-line multi-lens interferometers were successfully applied to phase contrast imaging and the study of coherence preservations by crystals, multilayers and refractive lenses.

The Mechanical Engineering group has undergone internal reorganisation, including the creation of a procurement unit, a 150 m^2 lab dedicated to precision mechanical assembly and a room for clean assembly, located within the experimental hall. In collaboration with beamline staff, this group has also been working on specific UPBL projects including:

UPBL11: Transfer of beamline from BM29 to BM23; installation of a new experimental table in BM23; design and procurement of the ID24 polychromators and mirrors.

UPBL10: Geometric acceptance test of a robotic arm for sample screening and data acquisition; detailed design of beam splitters and canted beam shutter; BM29 mirror design and purchase.

UPBL4: Design of the *NA* branch's double mirror (high stability requirements); refurbishment of the Kohzu double crystal monochromator for *NA*; detailed specifications of slits and absorbers.

UPBL6: Pre-design of the two spectrometers (high resolution IXS spectrometer and large solid angle IXS spectrometer); preparation of the move of ID20 to ID06 with a modification of the beamline layout and design of a double multilayer mirror.

A new concept for the positioning systems of long X-ray mirrors for the UPBLs and ID06 has been developed, optimised for high stability, low thermal drifts, and fine position control.

Computing Infrastructure

Investments into the computing infrastructure have been kept on a low level for much of the year awaiting the construction of the new data centre in the ESRF central building. With completion now being imminent, contracts have been placed for the network cabling, the water cooled racks, a large StorageTek tape library, and a new blade computing cluster. The new hardware will be installed at the beginning of 2011. The new blade cluster is based on a mixed architecture of graphical processor units (GPUs) and multi-core Intel CPUs with a large amount of random access memory. It will be used as a data analysis platform for the massive data flow generated by the tomography experiments. Similar systems dedicated to life science data analysis and simulation are planned in the course of 2011.

P. Elleaume, R. Dimper, H. Reichert, S. Pérez and J. Susini

Dynamics and extreme conditions

This year's Highlights again reflect the broad spectrum of scientific applications within the Dynamics and Extreme Conditions Group, and in particular underline the importance of continuously improving the instrumentation and of developing new concepts and ideas.

The first part of the chapter is dedicated to fundamental phenomena. The detection of superradiance and the collective Lamb shift combine beautifully the unique properties of synchrotron radiation, the X-ray wave guide effect and the ^{57}Fe Mössbauer resonance as a two-level system. This intricate setup enabled the detection of the predicted minute energy shift of 24 neV at 14.4 keV, corresponding to a relative change of $\Delta E/E = 1.7 \times 10^{-12}$! The second contribution reveals that the previously thought "homogeneous" supercritical phase of fluids can be partitioned into a liquid- and a gas-like portion, with the disappearance of the positive sound dispersion at THz frequencies marking the boundary between these two regions. The third contribution provides an important new insight into glass physics. High-resolution inelastic X-ray scattering measurements on hot vitreous silica clearly reveal two distinctly different scattering regimes of phonon-like excitations which are intimately related to the peculiar behaviour of the thermal conductivity and specific heat of glasses at low temperature.

The second part of the chapter focusses on high pressure studies. The first two contributions witness the significant progress made in the study of materials in laser-heated diamond anvil cells (DACs). Very tightly focussed and stable X-ray and laser beams, in conjunction with carefully designed diagnostic tools, are the pre-requisites for reliable and trustworthy results. The work on tantalum puts an end to a long-lasting controversy between previous experimental results and theoretical predictions and sets the standard for future work on the melting of solids. The knowledge of melting curves as a function of pressure is of utmost importance to constrain geochemical models and explains seismological observations. This is nicely demonstrated by the X-ray diffraction work on peridotite. In addition to these "static" measurements, the direct determination of sound velocities by inelastic X-ray scattering provides valuable complementary information, as shown in the highlight on the composition of the Earth's inner core. The last contribution illustrates that the combination of three experimental techniques – X-ray diffraction, X-ray absorption and conventional Mössbauer spectroscopy – were required to unravel the subtle interplay between structural, electronic, and magnetic degrees of freedom in delafossite, a binary transition metal oxide.

The third part of the chapter is devoted to the study of electronic and magnetic properties. The discovery of strong magnetic circular dichroism in K-edge resonant inelastic X-ray scattering (RIXS) opens exciting new perspectives in the study of magnetic materials, taking full advantage of the bulk-, valence-, and site-sensitivity of hard X-ray RIXS. The study of the spin reorientation transition of epitaxially grown Fe on W(110) illustrates the strength of nuclear resonance scattering to detect magnetisation directions with atomic layer resolution and a precision of a few degrees. "Classical" correlated electron systems such as V_2O_3 still offer new insights thanks to advanced spectroscopies.
A systematic study of the temperature, pressure, and doping dependence across the canonical Mott transition suggests that there might actually be two different mechanisms responsible for the metal-insulator transition. Finally, the X-ray Raman study on tetrahydrofuran clathrate hydrate formation gives a flavour of the kind of studies which will become routine once the IXS upgrade beamline UPBL06 becomes operational.

A significant amount of the experiments conducted on the beamlines rely on the excellent support services. The automatic diamond anvil cell gas loading system, the KAP surface at the lowest concentration of porphyrin solution. At somewhat higher concentrations, but still undersaturated, we enter the self-assembly regime. Here the islands show one preferred growth direction (**Figure 33a**) and grow together to form mono and multilayer structures. The step height of these structures is 2.5 nm, which corresponds to the planar porphyrin molecules lying perpendicular to the substrate surface. At higher concentrations, corresponding to a supersaturated solution, another stacked formation was found when more than 5 multilayers are formed. At these higher concentrations, the growth was no longer layer-wise, but nano-needles were formed, shown in **Figure 33b**. These nano-needles are oriented in the same direction, forming a single crystalline needle layer on the KAP surface. The molecular ordering in the nano-needles differs from that in the mono and multilayers. From the lattice spacing of 0.9 nm, as determined from X-ray diffraction, it follows that here the molecules are stacked in a tilted fashion, inclined by approximately 45 degrees. Both structures, the (multi)layers and the nano-needles, are oriented in one crystallographic direction over the whole substrate, which can reach an area of up to 1 cm^2. By using alternative organic crystals as substrates, the assembly can in principle be tuned to give organic crystal layers with unique electronic or photophysical properties.

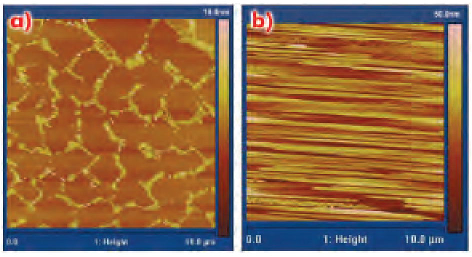


Fig. 33: AFM images of a) a honeycomb structure composed of oriented islands, b) nano-needle structure. The orientation of the porphyrin molecules in the nano-needles is determined via X-ray diffraction.

Structure and energetics of azobenzene on Ag(111): Benchmarking semiempirical dispersion correction approaches

Principal publication and authors
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M. Wolf (b,c), P. Tegeder (c),
F.S. Tautz (a) and K. Reuter (b,d),
Phys. Rev. Lett. **104**, 036102 (2010).
(a) Forschungszentrum Jülich (Germany)
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(c) Freie Universität Berlin (Germany)
(d) Technische Universität München (Germany)

Functional organic molecules at metal surfaces are studied because of their potential as a future molecular nanotechnology. A simulation platform is required that would allow the precise prediction of all relevant modes of the molecule-substrate interactions (chemical bonds of specific groups, Pauli repulsion, steric hindrance, and dispersion interaction). For this, the adsorption of organic molecules with highly polarisable conjugated ring systems on metals poses particular difficulties because the prevalence of dispersive van der Waals (vdW) interactions restricts the applicability of semilocal exchange and correlation (xc) functionals within density-functional theory (DFT). Since high-level theories that include nonlocal vdW interactions by construction are still barely tractable for large surface-adsorbed molecules, computationally inexpensive semi-empirical dispersion correction schemes to semi-local DFT (DFT-D) represent an appealing alternative. In these approaches, vdW interactions are considered approximately by adding a pairwise interatomic C_6R^{-6} term to the DFT energy. At distances below a cutoff, specified via the vdW radii of the atom pair, this long-range dispersion contribution is heuristically reduced to zero by multiplication with a short-range damping function.

The applicability of this DFT-D approach to organic molecules adsorbed at metal surfaces is uncertain. It is not clear how the results are affected by neglecting the screening of dispersive interaction between the adsorbate and more distant substrate atoms by the intervening metal layers. Moreover, adsorbate molecules, which also interact covalently with the substrate, exhibit bond distances that are so short that the uncertainties in the heuristic damping function of the dispersion term might mingle in an

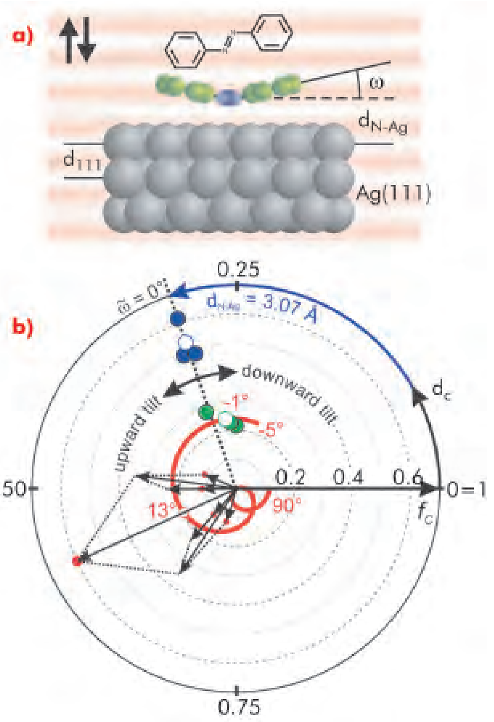

Fig. 34: a) Schematic adsorption model of azobenzene on Ag(111) in the X-ray standing wave field; b) Argand diagram of experimental coherent position d_c and fraction f_c for N1s (blue circles) and C1s (green circles). The red spiral represents the calculated d_c and f_c for C1s as ω sweeps from -5° to 90°; its intersection with experimental C1s data points defines the tilt angle of the phenyl rings.

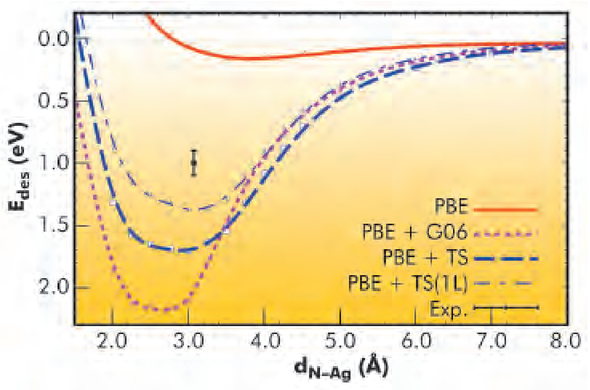

Fig. 35: Computed desorption energy curves and experimental point.

uncontrolled way with deficiencies of the employed semilocal DFT functional. Therefore, accurate experimental reference data are required to determine whether the improvements brought by including vdW interactions semi-empirically outweigh the aforementioned shortcomings.

We respond to this need by providing reference data for the molecular switch azobenzene on Ag(111) (Figure 34). The normal-incidence X-ray standing wave technique (NIXSW) at beamline **ID32** was used to determine key structural parameters of adsorbed azobenzene. Additionally, the desorption energy was measured by temperature programmed desorption (TPD). Employing a novel analysis scheme for NIXSW (Figure 34b), we extracted not only the height of azobenzene diazo-bridge $d_{N\text{-}Ag}$ that is straightforwardly accessible in NIXSW, but also the tilt of the phenyl rings ω. The derived structural data ($d_{N\text{-}Ag}$ = 3.07±0.02 Å and ω = -1±1.5°) demonstrate an essentially undistorted planar molecular geometry and agree well with the results obtained with DFT-D scheme due to Tkachenko and Scheffler (TS) [1]. Indeed, while the DFT-PBE strongly overestimates the diazo-bridge adsorption distance (3.64 Å) demonstrating the well-known incapability of semilocal xc functionals to account for long-range dispersive interactions, the tested DFT-D schemes by Grimme (G06) [2] and TS reveal a sizable reduction of $d_{N\text{-}Ag}$ to 2.75 and 2.98 Å (Figure 35). All three schemes predict almost flat molecular geometry in similar agreement with experiment.

Unfortunately, the improved structure in DFT-D goes together with a notable overbinding. Most probably the reason is the screening of dispersive attractions between the adsorbate atoms and more distant substrate atoms that is neglected in the strictly pairwise evaluation of the dispersion interaction as inspired by Hamaker theory. Mimicking this screening by reducing the number of substrate layers considered in the pairwise interaction C_6R^{-6} term to one and by even diminishing the C_6 coefficients of the Ag atoms in the topmost surface layer indeed shifts the computed binding energy curves closer to experimental values, but essentially without affecting the $d_{N\text{-}Ag}$ (Figure 35).

In summary, we demonstrate that the existing DFT-D schemes are not suitable to describe comprehensively the role of vdW interactions for adsorption at metal surfaces because screening effects are not (yet) considered. However, the insight that the adsorption geometries are less sensitive to the neglect of screening is intriguing. It suggests that these schemes may provide significantly improved structural data at zero additional computational cost. Such structures are then a useful starting point for higher-level theory, aimed at refined binding energies or a more comprehensive understanding of the adsorption system.

References

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[2] S. Grimme, *J. Comput. Chem.* **27**, 1787 (2006).

2010 manpower *(posts filled on 31/12/2010)*	Scientists, Engineers, Senior Administrators	Technicians and Administrative Staff	PhD students	Total
Staff on regular positions				
Accelerator and Source	30	37.4		67.4
Beamlines, instruments and experiments*	229	88.2	27.5	344.7
General technical services	28.6	51		79.6
Directorate, administration and central services	35.6	52.2		87.8
Sub-total	*323.1*	*228.8*	*27.5*	*579.4*
Other positions				
Short term contracts	6.8	12		18.8
Staff under "contrats de professionnalisation" (apprentices)		20		20
European Union grants				0
Temporary workers				0
Total	**329.9**	**260.8**	**27.5**	**618.2**
Absences of staff (equivalent full time posts)				23.6
Total with absences				*594.6*
Scientific collaborators and consultants	*9*			*9*
External funded research fellows	*3*		*24*	*27*

** Including scientific staff on time limited contract.*

Organisation chart of the ESRF

(as of January 2011)

Council
Chairman: J. Moulin
up to 3 delegates per Contracting Party

Administrative and Finance Committee
Chairman: N. Pratt

Science Advisory Committee
Chairman: R. Abela

Review Commitees
Chemistry-related studies - Chairman: S. Margadonna
Electronic and magnetic properties - Chairman: P. Strange
Crystals and ordered systems, structures - Chairman: S. Klotz
Disordered systems and liquids - Chairman: S. Magazù
Applied materials and engineering - Chairman: N. Zafeiropoulos
Environmental and cultural heritage matters - Chairman: M. Denecke
Macromolecular crystallography - Chairman: A. Leslie (temporary)
Methods and instrumentation - Chairman: C. Schroer
Medicine - Chairman: K. Engelke
Soft condensed matter and biological materials - Chairman: A. Petukhov
Surfaces and interfaces - Chairman: E. Garcia Michel

Director General
F. Sette

DG's Services:
- Head of DG's Office/Secretary of Council: I. Echeverria
- Communication Unit
- Business Development Office
- Internal Auditor
- Safety Group

ACCELERATOR AND SOURCE
Director: P. Elleaume

Theory and application software
Power supplies
Insertion devices
Front-ends
Radio frequency and linac
Diagnostics
Operation
Secretariat

ADMINISTRATION
Director: M. Rodriguez Castellano

Personnel
Finance
Purchasing

Joint ILL/ESRF Medical service

Joint ILL/ESRF Library

EXPERIMENTS
Director: S. Pérez

Beamline groups:
- Structural biology
- Structure of soft matter
- X-ray imaging

Director: H. Reichert

Beamline groups:
- Dynamics and extreme conditions
- Electronic structure and magnetism
- Structure of materials

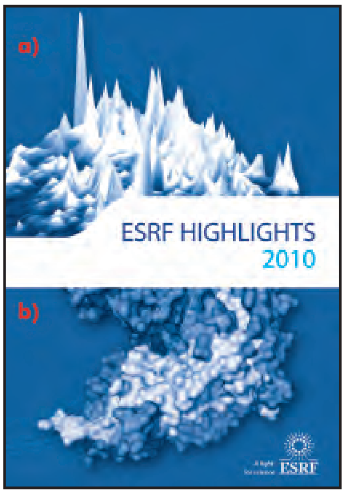
Scientific infrastructure
Theory
User office
CRG liaison
Secretariat

INSTRUMENTATION SERVICES AND DEVELOPMENT DIVISION
Head: J. Susini

Advanced analysis and modeling
Detector and electronics
Software
X-ray optics
Mechanical engineering

TECHNICAL INFRASTRUCTURE DIVISION
Head: R. Dimper

Management information systems and web
Systems and communication
Buildings and infrastructure
EX2/CPER project team
Survey and alignment
Vacuum



Cover

Design by M. Collignon. Featured images:
a) Imaging scale-free structural organisation of oxygen interstitial atoms in a high temperature superconductor, M. Fratini et al., page 114 (Credit: N. Poccia).
b) Crystal structure of the AHL acylase PvdQ from Pseudomonas aeruginosa, M. Bokhove et al., page 104 (Credit. M. Bokhove).

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