

PAUL SCHERRER INSTITUT



PSI Scientific Report 2006

Cover photo:

A razor-thin X-ray beam for sharp experiments is now available at the SLS POLLUX beamline.

(Photo: H.R. Bramaz)



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Paul Scherrer Institute, April 2007

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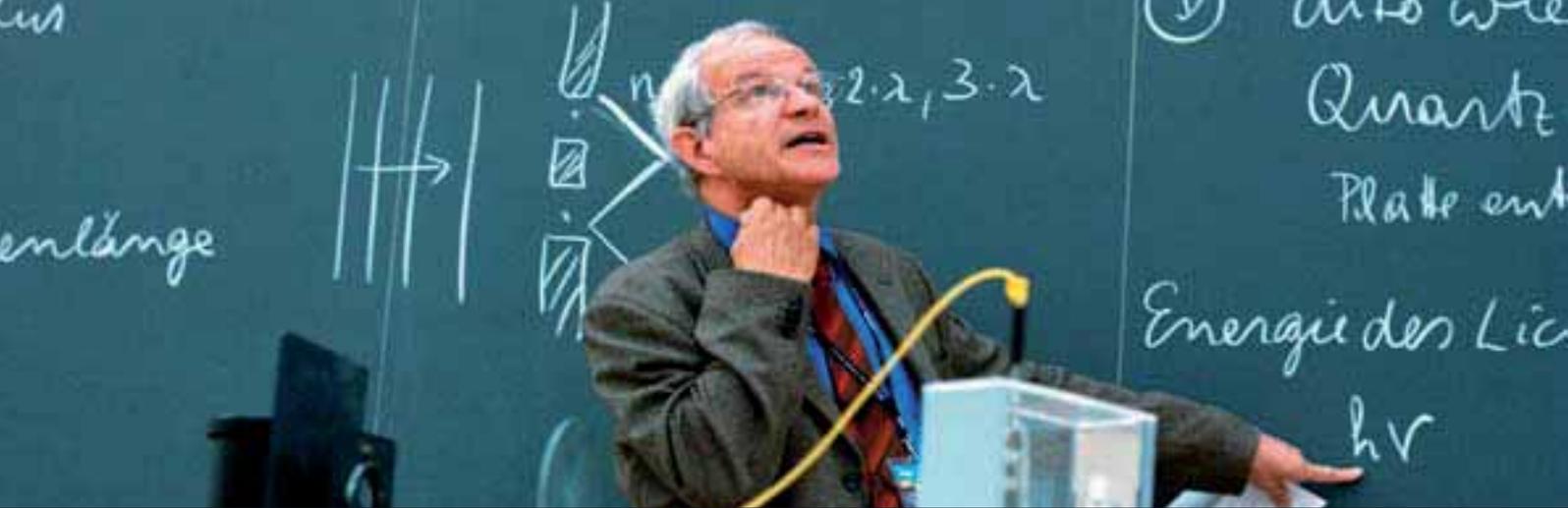
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It's all a matter of energy

Questions of energy – whether the physical energy that drives machines or the emotional energy that drives people – are important for society as well as the individual, for science as well as business. Electricity and oil companies have to be paid for the energy they provide and employees for the work they do. But how can the director of a research institute increase output when the energy input – in this case the PSI budget – is reduced? The solution of the ETH domain has been to define measurable short-term goals in order to increase efficiency. Since 2006 we have been working with target agreements and a small performance-related element in staff salaries.

For top-level motivation, however, that is not enough. Research needs more. Research is driven by visions, by belief in the future, by curiosity and the desire to contribute to the improvement of the world. The dream of discovery, of the breakthrough or key industrial application, does not always come true. Tenacity, patience and the courage to take unconventional paths are called for. All the more reason for gratitude, therefore, that in 2006 PSI achieved a number of internationally acclaimed successes and technological breakthroughs which had begun ten or more years ago as visions. It is these successes that continuously motivate our research and support teams to explore new avenues and invest their energies in the quest.

Milestone MEGAPIE

A high point of the neutron scattering program with the Spallation Neutron Source (SINQ) was the four-month long MEGA-

PIE experiment using a liquid metal target. The lead-bismuth target was bombarded with an 800 kW proton beam, achieving an up to 80% increase in the neutron stream compared with the earlier solid target. All SINQ instruments, including the new MARS spectrometer, profited from this increase.

Megapie also sets a technological milestone in the development of high intensity neutron sources for the transmutation of long-lived nuclear waste into short-lived isotopes. This new research perspective has excited great interest from a number of international partners in Europe, Asia and the USA, who have contributed both financially and scientifically to the success of the project (p. 104).

SLS besieged

Further facilities coming on stream at the Swiss Synchrotron Light Source (SLS) in the course of the past year included a beamline for X-ray microtomography in cooperation with the Swiss Federal Institute of Technology (ETH) in Lausanne. Working with the University of Erlangen, and funded by the German Federal Ministry of Education and Research, PSI also completed its POLLUX microscope line, as well as an instrument for experiments in time-resolved structure determination using ultra-short – 100 femtosecond (10^{-15} s) – hard X-ray pulses (p. 10).

PSI's two protein crystallography beamlines, which are among the world's best, are subject to intense time-pressure from the large number of users they attract. Here we have just

“Research is driven by visions, curiosity and the desire to contribute to the improvement of the world”, says PSI Director Ralph Eichler.

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overcome another technological hurdle, installing the first pixel detector with 6 million pixels, which will eventually replace the CCD-based detectors. Behind this quantum leap in data quality stand ten years of development on detectors for tracing charged particles in elementary particle physics.

We are particularly pleased that the intensive SLS use is creating a new competitive edge for all PSI departments, from biology to aerosol research and from catalytic converter development to a better understanding of the diffusion of radioactive waste in terminal storage facilities.

Sensational results and a new professorship

Independently, as well as in cooperation with ETH partners, PSI is conducting research into energy transformation efficiency in order to reduce both primary energy consumption and pollutant emission (p. 68). The scientific evidence that wood-burning stoves are responsible for a high proportion of particulate matter emission caused something of a political shock in this context (p. 126).

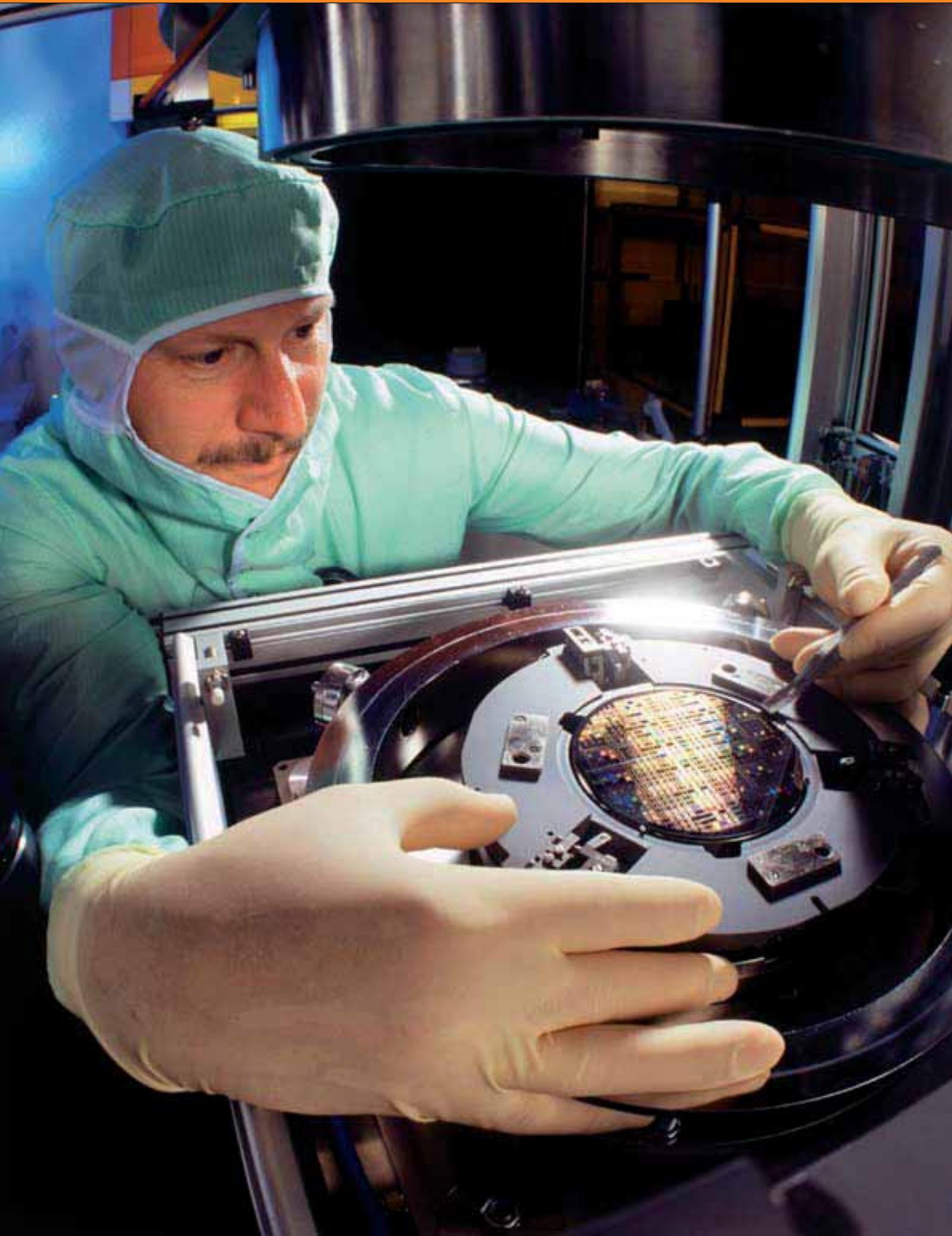
Proton therapy has also seen a number of technological breakthroughs in the past year. The new COMET superconducting cyclotron delivered a stable proton beam to GANTRY 1, and patient therapy could recommence in February 2007 (p. 58).

PSI was also voted by the international scientific community as Particle Therapy Co-Operative Group (PTCOG) centre. Our Institute has accordingly created a new professorship, affli-

ated to the University of Zurich, to boost medical research and strengthen teaching provision in this area.

PSI can be proud of its achievements in 2006. Therefore I would like to take the opportunity to thank all our colleagues here, and our partners at the universities and applied science institutes, as well as in the federal and Canton Aargau governments, for the energy they have made available to us in the form of highly motivated research and the funding of our mission.

Ralph Eichler, Director PSI



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Research in brief

Selected highlights in this year's report include muon spin studies and investigations of polymer films, the chemical properties of element 112 and the anti-tumour effects of radionuclides. In its fifth year of operation, results from the SLS include shedding light on superconductivity and understanding magnetism at the nanoscale. From the energy research departments we hear that progress has been achieved in the conversion of biomass to methane fuel, and towards the generation of hydrogen by solar thermochemistry. Combustion research, among other themes, focused on efficiency in gas turbine processes. Neutronic studies dealt with safety aspects of present nuclear reactors, thermal hydraulics with reactors of the future. Safety is also the issue in how ions migrate in waste repositories or in the operation of the MEGAPIE liquid metal target. The Competence Center Energy and Mobility of the ETH domain, for which PSI acts as the facilitator, started operation at the beginning of 2006, and several projects have been successfully launched.

The reports in this volume are only a fraction of the varied research undertaken at PSI in the past year; for more information visit our website – www.psi.ch

Nanotechnology developed at PSI has considerable potential for industrial use.

(Photo: H.R. Bramaz)

Ultra light science

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In 2006, the Swiss Light Source celebrated five years of operations. The facility produces ‘ultra-light’ science, in the sense that light is produced under ultra-stable conditions and put to use for example, ultra-fast time-dependent studies of matter in motion. The scientific weight of our user experiments, however, is anything but ultra-light; the SLS continues to shine with highlights in a variety of disciplines.

A brief history

The operation of the Swiss Light Source started mid 2001, when the materials science and protein crystallography beamlines saw the first light. Soon thereafter the beamlines for surface and interface spectroscopy and microscopy were put into operation. The SLS now has some ten beamlines operating, and will have 18 to 20 beamlines in 2011.

The SLS is the most advanced third-generation synchrotron light of medium electron energy (2.4 GeV) in the world. High intensity X-ray beams up to ca. 18 keV are produced on higher harmonics of small gap in-vacuum undulators. Closing of the undulator gaps down to 4-5 mm is made possible thanks to the highly optimized accelerator lattice design, combined with top-up injection of the electrons, which compensates for a possible decrease of the stored electron beam lifetime. Since many X-ray diffraction studies are performed in the range up to 20 keV, a medium-energy machine such as the SLS is competitive with the high-energy ones in many areas of science, against a fraction of their costs. Top-up injection is essential for another important reason. A constant stored current in the ring gives rise to a constant heat load on the ring chamber including the electron optical elements along its circumference. This has made the SLS a world champion in beam stability. The (generally) happy user may find out that the (almost) impossible experiment becomes possible.

The SLS users

The SLS is a user facility open to scientists from Switzerland and abroad. Two laboratories within the SLS are responsible for the operation and construction of beamlines. One laboratory (led by C. Quitmann) covers materials science, solid-state spectroscopy and microscopy, the other one (R. Abela) all

other disciplines, including detector development. The Laboratory for Micro- and Nanotechnology (J. Gobrecht) also belongs to the department operating the SLS and is fully integrated into the activities at the SLS.

Access to the SLS is provided through the selection of proposals for beam time by an international review committee. The selection is solely based on scientific merit. Currently, nearly half of our users are from the EU countries. Beam time at the SLS is heavily in demand, and Swiss scientists compete for access with the strongest user groups worldwide. Access by users from the EU is facilitated by the Integrating Activity IA-SFS of the FP6 programme of the EU. In addition to providing user support and constructing new beamlines, SLS staff members pursue research projects of their own. This is important for the local scientific culture and ensures user support of high quality. The SLS also provides services to industrial users. In 2006, ca. 10% of the total beam time has been sold to companies (mostly pharmaceutical) for proprietary research. Companies are charged for proprietary work on the basis of full cost recovery.

Mission

Our mission is to provide photon beams to researchers in the natural sciences. Our strategy is to excel in a number of selected disciplines rather than trying to serve the needs of all users. Major thrust areas are: structural biology, biomedical imaging, nanoscale magnetism, properties of correlated electron systems and pico- and femtosecond X-ray spectroscopy. Our R&D efforts in pixel detectors and X-ray optics are internationally well recognized. At one of the absorption spectroscopy beamlines, hard X-ray pulses of ca. 80 fs duration are generated by use of the electron beam slicing method. This is the world's brightest source of femtosecond hard X-ray

pulses (up to ca. 20 keV) until the X-ray free electron lasers in Stanford and Hamburg start operation and take over. SLS fruitfully collaborates with external groups which bring new instruments or methods to the SLS or act as ‘power users’. These groups contribute financially or in kind to the construction and running of beamlines.

The scientific output of the SLS grows in proportion to the number of beamlines in operation. In 2006, experiments at the SLS resulted in 220 publications, of which 28 appeared in top journals (Nature, Science, Cell, PRL).

Science

The research area currently with the highest impact is undeniably structural biology. In order to remain at the forefront, the SLS invests substantially in instrumentation and manpower. The beamlines for protein crystallography (PX-I and PX-II) are generally recognized as being among the world’s best in their kind. They attract internationally reputed structural biologists from academia as well as those from leading pharmaceutical companies. Roche, Novartis and the Max Planck Gesellschaft have jointly financed an entire beamline, including its operation. The biology groups from ETH, Swiss universities and the Bio Department at PSI are all important users. The SLS invests in innovative pixel detectors for PX, facilities for diffraction from micrometer-sized protein crystals, robotics and web-based services such as mail-in crystallography. A spin-off firm in pixel detectors (DECTRIS) has recently been founded.

Solid-state spectroscopy is also one of our priority areas. The beamline for surface and interface spectroscopy offers full control over the polarization of the XUV radiation and has a station for angle-resolved photoemission spectroscopy (ARPES). Swiss users investigate, for example, properties of correlated electron systems, including high T_c superconductors and oxides exhibiting colossal magnetoresistance. Competition worldwide is severe. The SLS now invests in an upgrade of the ARPES station so as to make it the world’s most advanced beamline of its kind. An important new tool is the beamline ADRESS for high-resolution resonant inelastic X-ray scattering (i.e., Raman spectroscopy with X-rays), which starts operation in 2007. In addition, a facility for IR-spectroscopy will soon become available.

Another important topic is the dynamics of nanoscale magnetic systems on a picosecond time scale, for which the SLS offers a unique measurement platform. Orbital and spin ordering in metal-oxides are investigated using resonant soft X-ray scattering.

The beamline for materials science and tomography attracts a wide range of users. Unique is time-resolved (millisecond) powder diffraction using a strip detector developed in-house.

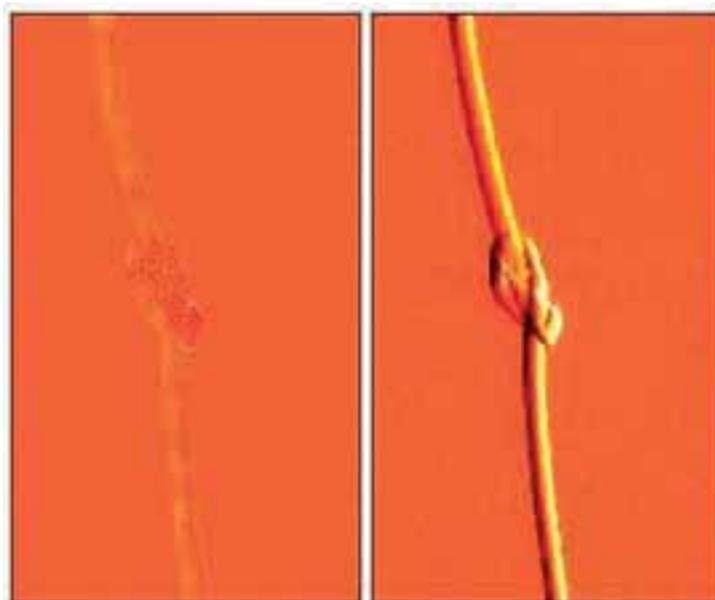


Figure 1: X-ray radiography of a knotted human hair: left with absorption contrast, right in phase contrast.

The facility is complementary to that at the Swiss-Norwegian beamline at ESRF.

X-ray absorption spectroscopy (XAS) using a microfocus beam is much in demand by chemists and environmental scientists. The beamline LUCIA, operated jointly with CNRS/SOLEIL, offers unique facilities for microXAS and X-ray fluorescence in the difficult photon energy range of 0.9 to 6 keV. It also attracts geophysicists studying condensed matter under high pressure. The beamline microXAS is used for studies of radioactive samples and for pump-probe studies of the dynamics of molecules in solution (EPFL).

For the period 2008-2011, the following major thrust areas have been defined: firstly femtosience with X-rays and secondly life sciences, in particular structural biology and bioimaging on all relevant length scales. Regarding the latter area, a third beamline for protein crystallography including a platform for on-site crystallization is under construction. Furthermore, a beamline for tomography and medical radiology will be dedicated to imaging on (sub-)micrometer and small-animal length scales (with EPFL). IR-microscopy is in development, as is a facility for solution scattering and coherent scattering at the beamline cSAXS.

The SLS has a bright future for years to come!

Seeing matter within a picosecond

Gerhard Ingold, Paul Beaud, Steve Johnson, Rafael Abela, Dirk Abramsohn, Faton Krasniqi, Thomas Schmidt, *Research Department Synchrotron Radiation and Nanotechnology, PSI*; Andreas Streun, Volker Schlott, *Department of Large Research Facilities, PSI*; Daniel Grolimund, *Research Department Nuclear Energy and Safety, PSI*

A tuneable undulator source for femtosecond X-rays in the range 4 – 12 keV is now in operation at the SLS storage ring. The source combines accelerator and laser technology relevant for the next generation light sources. It provides an inherently synchronized femtosecond laser ‘pump’ and X-ray ‘probe’ to enable time-resolved absorption and diffraction experiments. Observation of coherent optical phonons in bismuth single crystals via X-ray diffraction demonstrates the excellent spatial and temporal stability of the source that allows direct quantitative measurement of ultrafast lattice dynamics and associated phase transitions.

Relativistic electrons accelerated in vacuum emit synchrotron radiation. The frequency, polarization, coherence and time structure of this light can be precisely tailored by controlling the electron dynamics in phase space. ‘Laser seeding’ has originally been proposed to induce an energy modulation of the electron bunch to generate fully coherent light in a single pass Free Electron Laser (FEL). Later it has successfully been demonstrated [1,2] that this method can also be used to generate femtosecond soft X-rays in a storage ring [3]. Based on short-period in-vacuum undulator technology we extended this work into the Å-range [4]. The source is designed for femtosecond laser/X-ray pump-probe experiments in absorption [5] and diffraction over many shots to compensate for the low fs X-ray flux. It profits from the highly stable operation of the SLS storage ring with fast orbit feedback in top-up mode.

FEMTO source

The sequence of magnets installed at the μ XAS beamline, shown in Figure 1, acts as a 3-stage spectrometer. The 100 fs energy-modulated satellite electrons are generated along the laser/e-beam interaction region inside the modulator (wiggler). The modulated electrons are then separated from the core beam due to the dispersion provided by a chicane followed by refocussing magnets [6]. The X-rays are finally generated inside the narrow gap radiator (undulator). Photon absorbers and slit systems in the beamline suppress background radiation from the core beam.

The laser system consists of a femtosecond Ti:Sapphire oscillator synchronized to the SLS storage ring followed by two regenerative amplifiers. They are operated in parallel to deliver high energy femtosecond pulses for pumping samples and for modulating the electron bunches inside the storage ring to generate the femtosecond X-ray probe pulses. Coherent



Figure 1: FEMTO facility installed in the SLS tunnel.

synchrotron radiation emitted at the first dipole downstream from the radiator is used as an on-line diagnostic to optimize the energy modulation [7]. The operation of the FEMTO source is fully compatible with regular user operation through application of a hybrid bunch filling pattern.

The sliced X-ray photons are detected using an avalanche photodiode. A maximum sliced X-ray flux of $2 \cdot 10^5$ ($6 \cdot 10^4$) ph/s/0.1% BW was measured at 5 (8) keV. The suppression of the 100 ps core beam is better than 1000:1. The background is instead limited by a halo of surviving previously modulated electrons that limits the signal-to-background ratio to approximately 50:1.

Coherent lattice motions in bulk bismuth

First diffraction experiments on Bi single crystals – measured at 7.1 keV with a bandwidth of 1% – show evidence of high amplitude coherent optical phonons similar to those observed in [8] and also recently measured at the Sub-Picosecond Pulse Source (SPPS) in Stanford [9]. By fitting this data to a simple model of a displacive excitation (red curve in Figure 2) we obtain an average phonon frequency of 2.60 ± 0.05 THz and an effective time resolution of 200 ± 20 fs. Deconvolution yields an estimated X-ray pulse width of 85 ± 50 fs.

In December 2006, we performed a systematic study of the lattice motions associated with coherent optical phonons as a function of pump fluence and probe depth. For over a week data could be accumulated with stable X-ray flux and overall timing drifts significantly below 100 fs. As an example, Figure 3 shows a demonstration of optical control of coherent lattice motions by applying a sequence of two identical pump pulses with a variable temporal separation, previously indirectly observed through reflectivity changes in the optical frequency domain [10]. Figure 3 depicts, to the best of our knowledge,

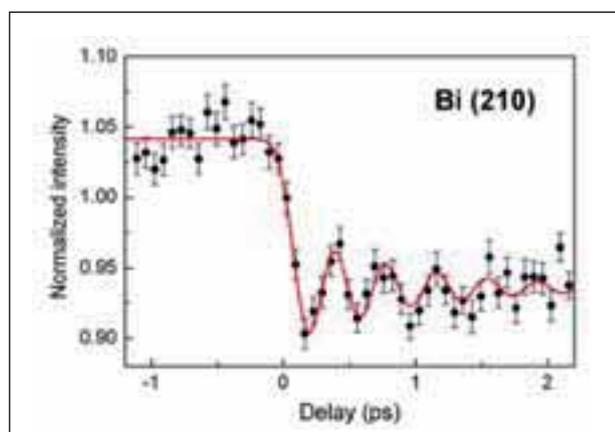


Figure 2: **Integrated diffracted intensity from the bulk Bi (210) reflection as a function of time after excitation with a pump fluence of 2 mJ/cm^2 .**

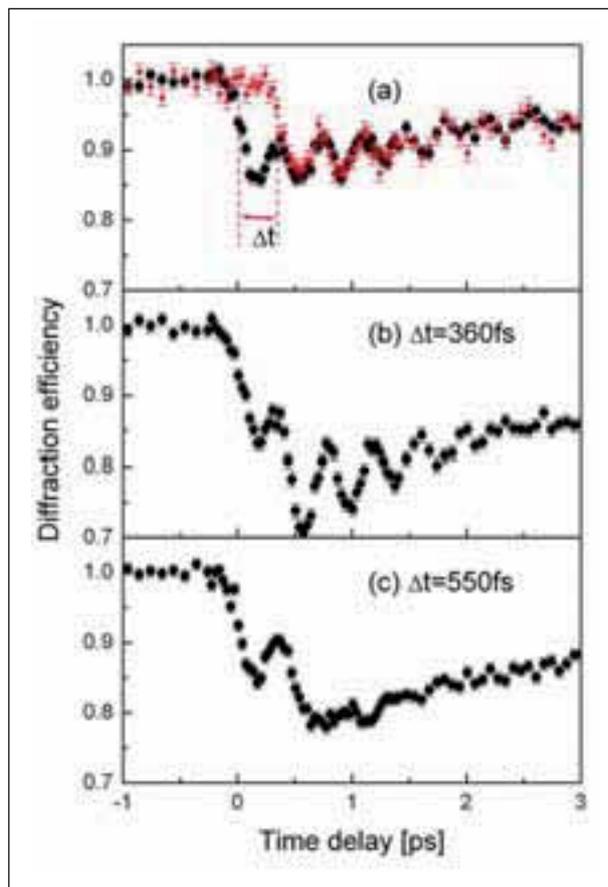


Figure 3: **Integrated diffracted intensity from the bulk Bi (111) reflection versus delay of the pump laser for single pulse (a) and double pulse excitation (b). Depending on the delay Δt between the two excitation pulses the coherent phonon motion can be amplified (b) or cancelled (c).**

the first optical control experiment where the coherent structural response has been probed directly with hard X-rays with femtosecond resolution.

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Making the invisible visible

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Seeing the invisible has always been a driving force of human development. Ever since Galileo Galilei and Anton van Leeuwenhoek built their first telescopes and microscopes, discoveries benefited from new instruments. In the old days these were glass lenses allowing the refraction of rays of visible light and creating magnified images visible to the eye. Today we want to see using X-rays. X-rays are nothing but light waves with a 100 or 1000 times smaller wavelength. No wonder they need different tools and that X-ray lenses look nothing like a magnifying glass. They are tiny objects made possible by nanotechnology.

At PSI many scientists are working on the fabrication of light forming objects for X-rays and are applying such objects to the X-rays produced by the Swiss Light Source (SLS) to make the invisible visible.

Shaping the light is a must in a microscope whether it is operated with visible or with X-ray light. However X-rays are much more difficult to shape because unlike visible light there is no material which is transparent and at the same time has sufficient refracting power for an X-ray beam. The refractive index which is typically 1.5 for glass and visible light is extremely close to unity (~ 0.999999) for X-rays. A centimeter-sized X-ray lens would thus have a focal length of kilometers, very im-

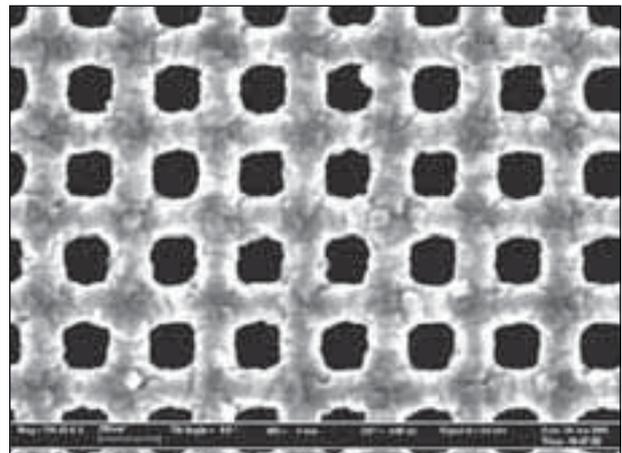


Figure 2: Nano-sieve made out of aluminium acting as a very effective filter transmitting only wavelengths comparable to its period [2].

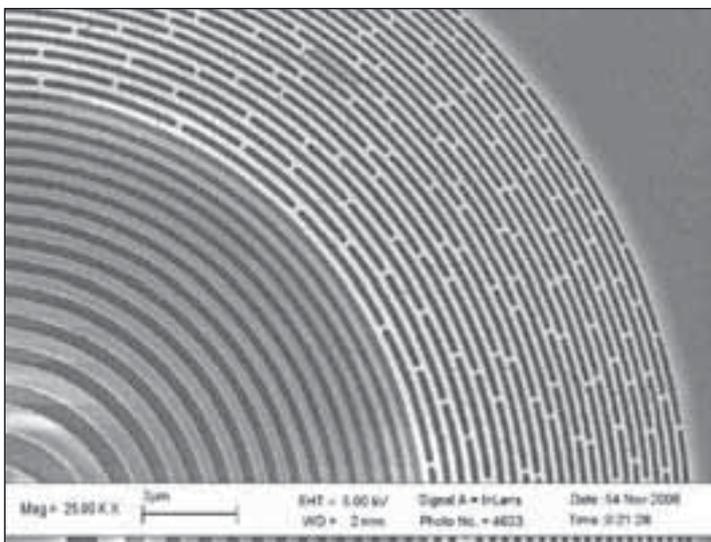


Figure 1: Fresnel zone plate acting as a lens for X-rays. The outermost and thinnest line is only 50 nm wide and is stabilized by bridges preventing it from collapsing.

practical for a microscope. Therefore, X-ray optics have to take advantage of diffraction and need to have structure sizes comparable to the wavelength λ which is nanometers (1 nm = 0.000000001 m) for X-rays.

Diffractive X-ray lenses, also called Fresnel zone plates, are made of tiny concentric rings with well controlled diameter and width [1]. An example is shown in Figure 1. The rings are very narrow (down to 50 nm) and the trenches relatively deep (1000 nm). Translated to a human scale this would correspond to a dam only 50 cm wide, but with a 10 m trench on either side. Therefore the rings are stabilized by radial bridges. Such Fresnel zone plates are to X-rays what a glass lens is to visible light. They allow focusing and thus magnifying objects invisibly small to the human eye.

Nano light sieve

Once able to control X-rays they can be put to work. An example is lithography where X-rays, due to their short wavelength λ , allow the fabrication of unbelievably tiny structures over large areas as shown in Figure 2.

Here a nano-sieve has been produced [2]. The holes in this sieve should allow light to pass through, while the aluminium wires are expected to block it. But testing this led to a surprise: for light of a wavelength comparable to the period of this nano-sieve ($\lambda = 350$ nm) much more light passes through than expected. The incident light excites so called plasmons in the aluminium wires resulting in 140% light transmission through the sieve. The sieve acts as a funnel, but only for a selected wavelength. When making structures sufficiently small to become comparable to the wavelength, one is thus able to create filters which allow certain wavelengths (or colours) of the light to pass, while they very efficiently block others.

Having learned how to manipulate X-rays one can now build a microscope and put them to use. Figure 3 schematically shows the setup used at the new POLLUX beamline. Here a Fresnel zone plate focuses the light to a tiny spot only 50 nm (0.00005 mm) in diameter and a thin sample is raster scanned through this X-ray focus. The transmitted light is detected and its intensity is plotted as a function of position $I(x,y)$ using a computer. Such X-ray microscopes not only make nano objects visible, they also provide information on their chemical composition.

A single 200 nm aerosol particle is seen to consist of an organic shell composed of organic material (adipic acid) covering an inner core of ammonium sulfate (NH_4SO_4), see Figure 4.

Making such surface coating visible is important because the surface is what matters for chemical reactions in the atmosphere and for the radiation balance of our earth, which is currently in focus because of the greenhouse effect. Seeing such particles, which are invisible to the eye, allows the investigation of their role in atmospheric chemistry and climate change.

Seeing without lenses

Although imaging usually requires manipulation of the light using objects such as lenses or Fresnel zone plates, scientists have found ways around this. They can now produce images entirely without lenses.

For this the unique properties of modern synchrotrons like the SLS are needed. These high-tech lamps emit X-rays coherently, meaning that all rays have a fixed relation of their wave crests and valleys. If such coherent rays illuminate an inhomogeneous sample the rays are deviated differently de-

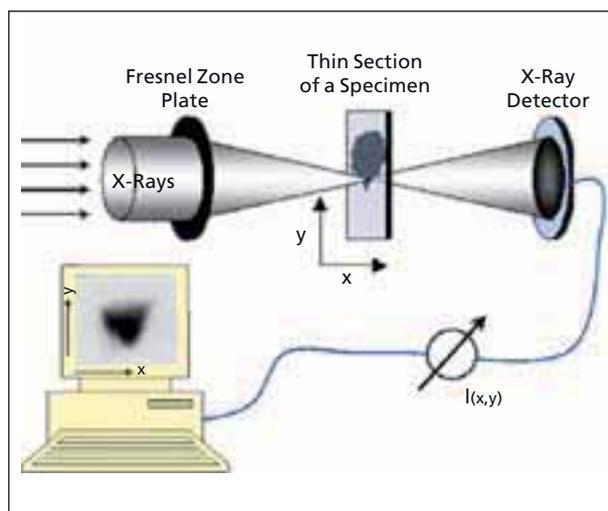


Figure 3: **Sketch of a scanning transmission X-ray microscope (STXM) showing the image of a 200 nm aerosol particle on the screen.**

pending on sample thickness, composition, etc. Wave crest and valleys of the outgoing rays therefore no longer have a fixed relation. When two or more such rays are now superimposed on the detector, the waves of the rays add up or cancel out depending on the relative position of crest and valley. Adding two crests increases the intensity, while adding crest and valley results in zero intensity.

This superposition thus transfers information from the sample to the detector. Such superposition images are not directly understandable for the human eye, yet since the process leading to their formation is mathematically well understood,

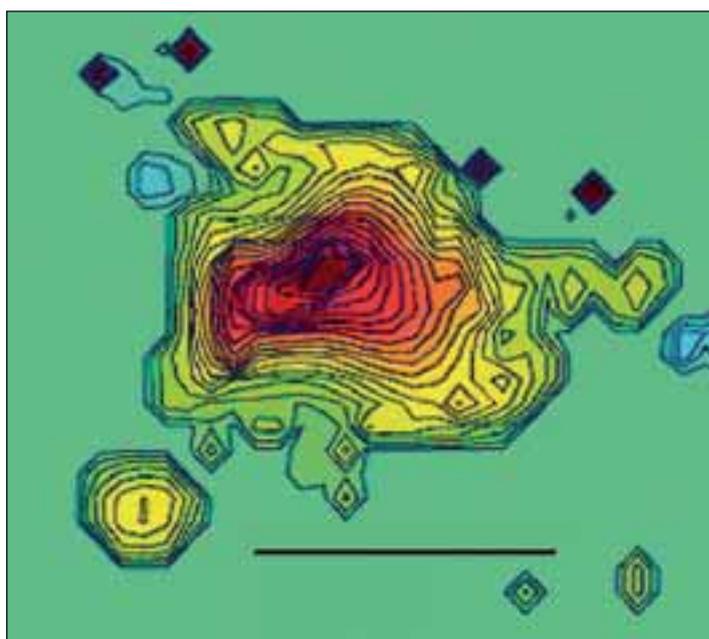


Figure 4: **Spectroscopic image of a 200 nm aerosol particle showing ammonium sulfate in red (core) and adipic acid in yellow (shell).**

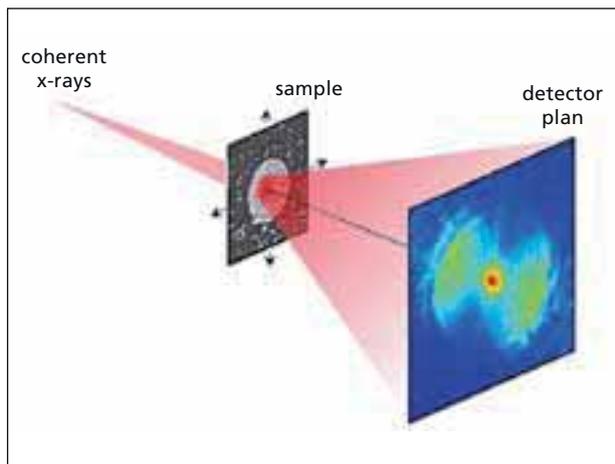


Figure 5: Sketch of a lensless imaging experiment showing the sample illuminated using coherent X-rays and the diffraction image produced on the detector [3].

they can be reconstructed using modern computer algorithms.

A sketch of such a lensless imaging experiment is shown in Figure 5 [3]. The sample is illuminated by the coherent X-ray beam and changes the position and amplitude of the X-ray crests and valleys. On the detector the rays are superimposed resulting in an image. Because the sample can be moved and many such images can be stitched together the data contain redundant information. This so-called oversampling allows reconstruction of the sample properties in the computer. Figure 6 shows first results of this new technique on a test object, a Fresnel zone plate. This is a particularly good object since its shape is a well-known pattern and thus allows testing of the smallest structures visible using this new lensless method. To add further test objects it is additionally decorated with tiny gold nanospheres. Figure 6 compares a traditional electron microscope image (a) with an image obtained using lensless X-ray imaging (b). The red circles indicate the many shifted areas of X-ray exposure. Figure 6b is the recon-

structed image from lensless imaging. The test object is well visible and even individual gold nanospheres are easily identified. This proves that vision without lenses is possible. The smallest structures clearly visible are only 100 nm wide, as shown in the inset.

The future is bright

Considering that these images are the first ever obtained using this lensless X-ray imaging, the future looks bright for microscopy using X-rays but doing away with lenses and instead relying on coherent illumination and powerful computer reconstruction.

For centuries humans have tried to get deeper insights into the world surrounding them. They have developed tools such as lenses and microscopes allowing them to study ever smaller objects. Using modern synchrotrons such imaging can be performed with X-rays, thus giving even deeper insight into matter. But we are on the way to going even further. Imaging without lenses has been demonstrated. This is a tool which opens a whole new view for science and will find broad applications in many fields ranging from fundamental physics to materials science and biology. Let's see what we will discover next.

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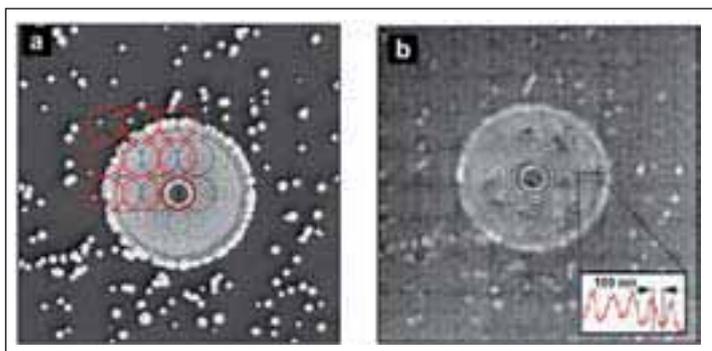
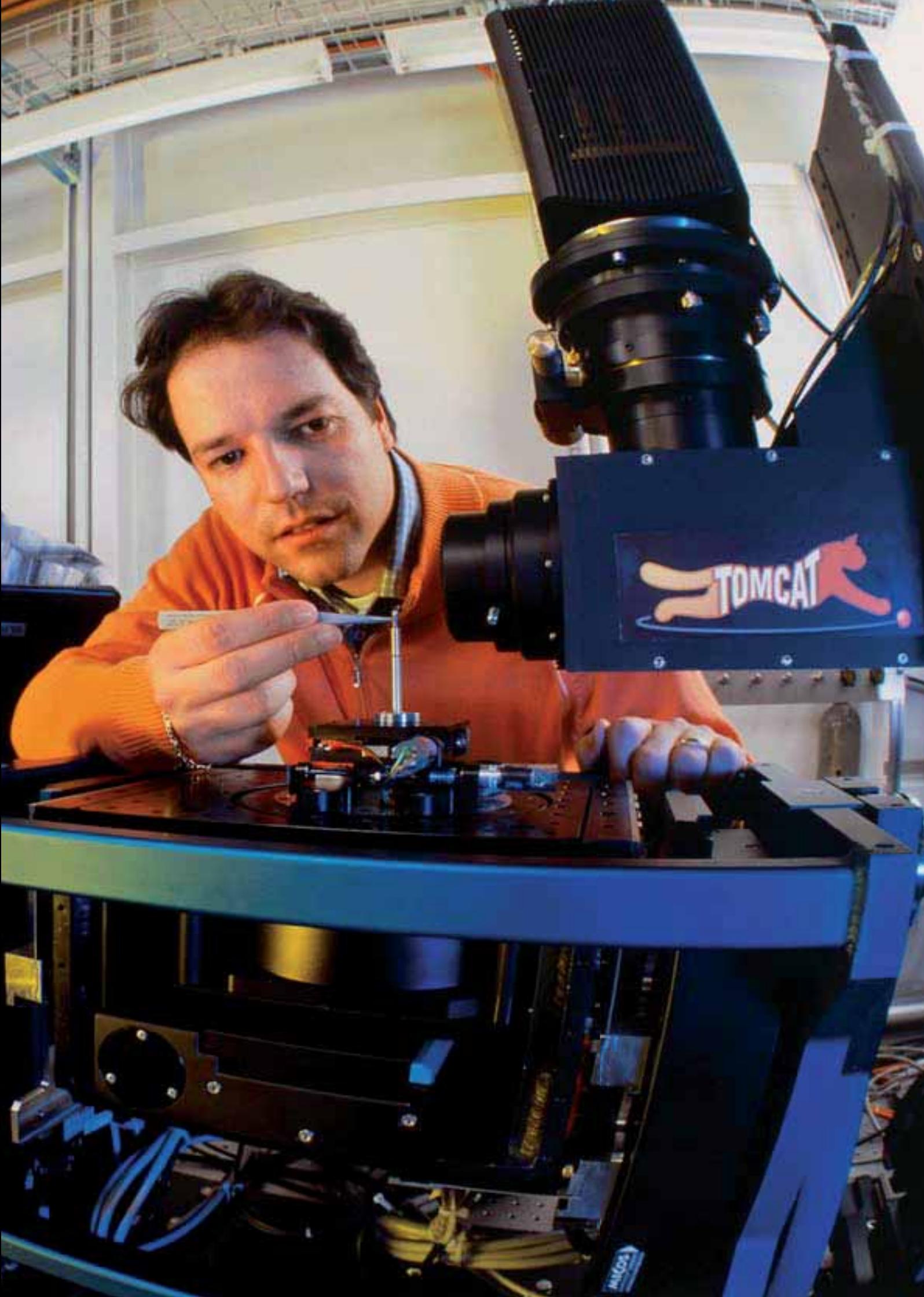


Figure 6: Scanning electron microscope image of the test object (a Fresnel zone plate) with red circles indicating the overlapping exposure areas used for theptychographic reconstruction (a) and the reconstructed image obtained by lensless imaging (b) with a spatial resolution of below 100 nm [3].

Figure 7: An experiment is set up at the new TOMCAT beamline. (Photo: H.R. Bramaz)



Magnetism under the spotlight

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With the need to produce electronic devices which are smaller, faster and cheaper, the pressure is on the magnetism community to come up with new technologies for data storage and manipulation. This requires a detailed understanding of magnetic behaviour at the nanoscale, needing both state-of-the-art techniques to manufacture small magnetic elements but also to analyse the detailed magnetic spin configurations. This year we have made progress in several areas, uncovering the nature of antidot arrays and magnetic domain walls in nanowires. The images of the magnetic spin configurations not only reveal information about the fundamental physics involved but are also beautiful to look at.

Smaller, faster, cheaper! So is the cry from the magnetic recording industry. And rightly so. In the age of laptops, mobile phones and MP3 players, where it has become essential to gain fast access to memory-devouring data such as cinema films or home videos, we need to find new ways to increase data storage capacities and speed up data transfer. This in-

evitably leads to a push of magnetic technology, currently used for data storage in a computer hard drive, down to the nanoscale. But before we can create these new technologies, we need to understand the detailed behaviour of magnetic systems at such small length scales. A very powerful method to do this is direct imaging of magnetic spin structures using the photoemission electron microscope (PEEM) at the SLS, which has been running for 5 years and each year has produced exciting new information. Of course, we need to be able to manufacture such small elements, and at the Laboratory for Micro- and Nanotechnology we have leading facilities for fabrication of magnetic nanostructures. In the past year we have uncovered the behaviour of magnetic domain walls in nanowires and determined the domain configurations in antidot arrays. Naturally, all this would not have been possible without the highly productive collaboration with another leading group in nanoscale magnetism at the University of Konstanz, and the expert support in micromagnetic simulations at the University of Salamanca.

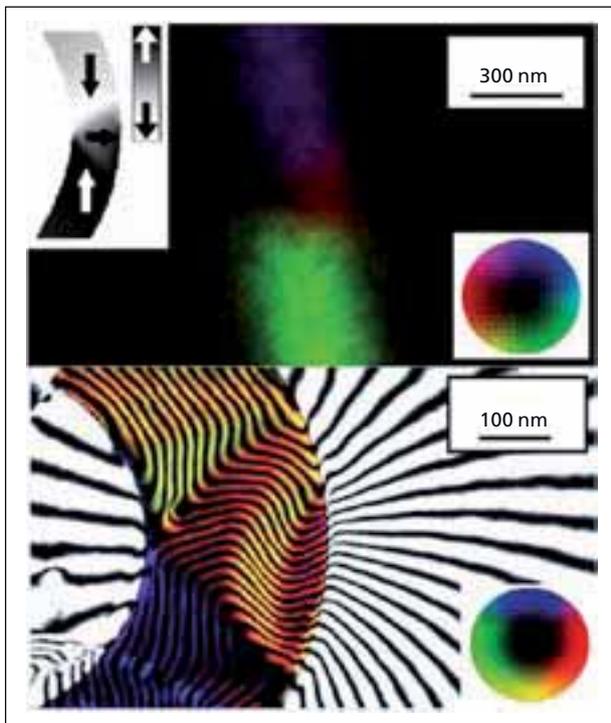


Figure 1: **Magnetic spin configuration in a transverse domain wall (a) imaged with PEEM and (b) with electron holography (Rafal Dunin-Borkowski, Cambridge).** Colour wheel: orientation of the spins.

Domain wall pinballs

Magnetic domain walls are simply the boundary between two magnetic domains with magnetic spins pointing in different directions. It has been known since the early 20th century, in the days of the great magnetic expert, Louis Néel, that it is possible to affect magnetic domain structures and therefore to move domain walls using a magnetic field.

However, 20 years ago Berger touched upon the idea of moving domain walls in a nanowire with an applied current. With

the improvement in nanoscale fabrication and characterization, such effects have become measurable and there has been an explosion in scientific activity with the promise of startling new data storage technology based on manipulating domain walls with currents, like pinballs.

This year we have shown both the thermal behaviour of these domain walls with the PEEM and the effect of the stray field coupling between them, akin in the macroscopic world to bringing two magnets together [1]. In addition, we are working hard to determine the key effects behind current-induced domain wall motion [2]. Our collaboration was in fact one of the first to directly image the domain wall movement due to spin-current injection and to show the important influence of the domain wall structure on the speed of the domain wall movement.

Carpet of magnetic colours

Could Néel have anticipated in 1944 that his prediction of how magnetic domains form around a cavity would provide inspiration in the nanoworld to use tiny holes as building blocks to engineer magnetic properties? We now have the ability using electron beam lithography to produce Néel's cavities with nanoscale dimensions in ferromagnetic thin films, arranging them very precisely in a regular pattern in a cobalt film with periods down to 100 nm [3].

These so-called antidot arrays have new and fascinating properties; Figure 2 shows a two-dimensional map of the magnetic spins in one of the antidot arrays with a period of 1 μm . At first sight, the image is reminiscent of a carpet with an intricate, unfathomable design. Taking a closer look, we can identify chains of magnetic domains, given by lines of colour running vertically (magnetic spins pointing upwards or downwards) or horizontally (magnetic spins pointing to the left or to the right). On application of a magnetic field, we observed the details of the way in which the system switches in an applied magnetic field from one magnetic state to another, which is important for the control of new magnetic devices. Comparing our PEEM observations with micromagnetic simulations and magneto-optical Kerr effect measurements, we were then able to identify the key mechanisms responsible for the observed behaviour. It turns out that on application of a vertical magnetic field, the switching from all magnetic spins pointing up to all spins pointing down (a change in colour from green-yellow to blue-pink in the figure) occurs by nucleation and propagation of vertical chains of domains. The vertical domain chain configuration (chain length and position) at each field value, and therefore the instantaneous colour design of this magnetic carpet, is highly dependent on the presence of the horizontal domain chains. The micro-

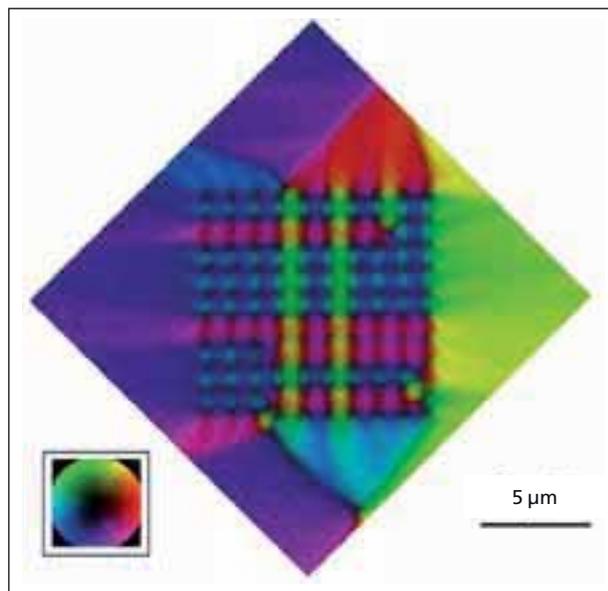


Figure 2: **Magnetic spin configuration in an antidot array.** The colour wheel indicates the spin orientation.

magnetic simulations helped to explain this behaviour; the ends of orthogonal chains prefer to coincide because they form a stable domain wall configuration and as the vertical chains grow, the moving chain end is blocked on approaching a horizontal chain due to the formation of high angle domain walls. The ability to trap the domain walls is potentially interesting for engineering of new magnetic nanoscale devices that exploit domain walls to store information or perform logic operations. Not only is it possible to spatially modulate the ferromagnetic properties of a thin film by introducing an array of holes, but also by coupling it to an array of ferromagnetic elements with different properties [4]. With a variety of methods to change the function of magnetic thin films and multilayers, we are set with a nanofabrication toolbox to address the data storage problems of the future.

The uncovering of the nature of nanoscale magnetic elements has only been possible due to the fruitful collaboration with S. Czekaj, C. A. F. Vaz, J. A. C. Bland, R. J. Matelon, U. G. Volkmann, P. Fischer, M. Horisberger, R. E. Dunin-Borkowski, A. Hoffmann, J. E. Pearson, and J. Brugger.

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Shedding light on superconductivity

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Arguably one of the top intellectual challenges facing solid state science is the question of the mechanism of high- T_c (critical temperature) superconductivity. Both their unusually high T_c s and their perhaps even more unusual normal state properties have conspired to make the cuprate high- T_c superconductors among the most intensively studied solids in existence. Photoemission spectroscopy has played a very important role in their investigation over the last twenty years, as it offers a direct window on the character and dynamics of the low-lying electronic states responsible for superconductivity.

Milestones along the photoemission path [1] have included determination of their Fermi surface topology and form, the anisotropic energy gaps related to their d -wave superconducting order parameter and the existence of a pseudo-gap in their normal state. The drosophila for high- T_c photoemission investigations is the bilayer system $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, or Bi-2212 for short. This system is such a favourite because it delivers excellent cleavage surfaces and has a high T_c (maximally 95K). Considering the fact that the topology and shape of the Fermi surface is a basic characteristic of every metal, it was a highly remarkable situation that until now the origin of one of the two primal Fermi surface features of Bi-2212, namely its shadow Fermi surface (SFS), was still not understood. Here, we briefly relate how the circle has been closed, from the Swiss discovery of the SFS in 1994 [2], to how the strengths of the SLS could be harnessed to finally dispel the shadows surrounding this phenomenon.

Figure 1 shows a simplified schematic of the Fermi surface of a modulation-free sample of Bi-2212. The black box shows



Figure 1: **Schematic of the main (red) and shadow (blue) Fermi surface in Bi-2212 high- T_c superconductors.**

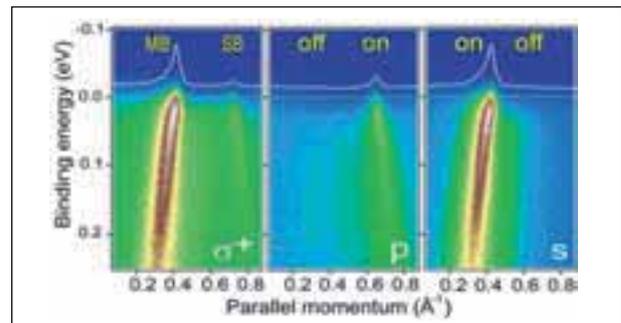


Figure 2: **Polarisation dependent ARPES data along the nodal (ΓY) k -space direction in Bi-2212.**

the commonly used (tetragonal) Brillouin zone, and the red (blue) circles represent the main (shadow) Fermi surfaces. The ΓM direction is parallel to the Cu-O bonds in the CuO_2 planes of the superconductor, whereas ΓY and ΓX have the nickname ‘nodal’ directions, as at these points on the Fermi surface the superconducting energy gap has its node.

The data that gave us the first clue as to the microscopic origin of the SFS are shown in Figure 2. Plotted is the photoemission intensity (colour scale) with binding energy on the y-scale (zero is the Fermi energy) and crystal momentum (or wave vector) on the x-scale, in this case along the ΓY nodal direction.

Advantages of the SLS

These data exploit one of the advantages of synchrotron radiation from the SLS: its variable polarisation. The left-hand panel is recorded with circular polarised light (σ^+), the centre panel with p-polarised light and the right panel with s-po-

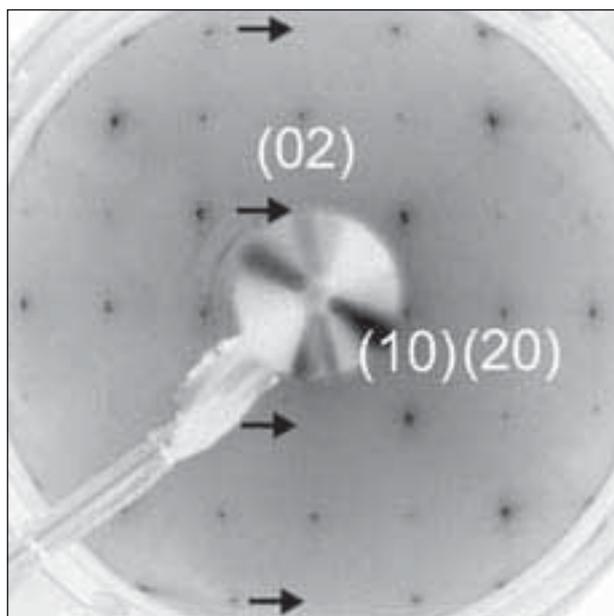


Figure 3: LEED image taken from the (Pb,Bi)O termination layer of a twin-free (Pb,Bi)-2212 high- T_c superconductor.

larisation. The σ^+ data show first the main band (labelled MB) and then, weaker, the shadow band (labelled SB). The big surprise was that s(p)-polarisation only shows the main(shadow) bands, never both together. This is clear evidence that the main and shadow states have different, in fact *opposing*, mirror symmetry with respect to the ΓY line in k -space. Intriguingly, along the ΓX nodal direction, both s (on-on) and p-polarisation (off-off) give the same behaviour for both main and shadow states.

Electron diffraction data

How can a supposedly tetragonal crystal support states with different symmetries along the two Brillouin zone diagonals? The answer came from electron diffraction data from modulation- and twin-free Pb-doped Bi-2212 crystals grown in the Amsterdam mirror furnaces. These display characteristic extinctions (missing spots) in the LEED patterns. These missing spots (marked with arrows in Figure 3) can be attributed to ($\emptyset = \text{zero}, k$) reflections (k being odd) within an *orthorhombic* unit cell. These systematic absences in the LEED pattern do not come about simply because the lattice constants a and b are not equal, but arise from a significant shift of an atom from its tetragonal position, such as the displacement of the central atom shown in Figure 4. The red ball represents the undistorted, tetragonal position and the offset, blue ball the displaced orthorhombic position.

The orthorhombic symmetry and the atom displacements are also found in high-quality single-crystal X-ray and neutron diffraction data [3]. These orthorhombic displacements mean

that the only remaining mirror plane is the xz plane (relevant for nodal ΓX data); the diagonals are no longer crystalline mirror planes at all and there is now a glide plane running parallel to yz (relevant for nodal ΓY data). It is this glide plane that is responsible for the parity flip seen in the photoemission data [4].

Thus, the shadow Fermi surface chapter in the Bi-based high- T_c superconductors can finally be closed. We prove that the shadow Fermi surface has nothing to do with short-range antiferromagnetic spin correlations, but is rather due to orthorhombic displacements of atoms from the ideal tetragonal positions (both in the Bi-O planes and to a lesser extent in the CuO_2 planes). This causes a back-folding of bands within the new, smaller orthorhombic Brillouin zone, and gives the bands different mirror symmetry in the ΓY and ΓX Brillouin zone quadrants. The fact that these distortions are felt strongly by the Cu-O derived electronic bands, and even influence the mirror symmetry of these states, illustrates that the canonical Brillouin zone and Fermi surface for the Bi-based high- T_c need to be revised. The only experimental challenge remaining would be to detect the hybridisation gaps opening up where the ‘main’ (red) and ‘shadow’ (blue) Fermi surfaces shown in Figure 1 intersect.

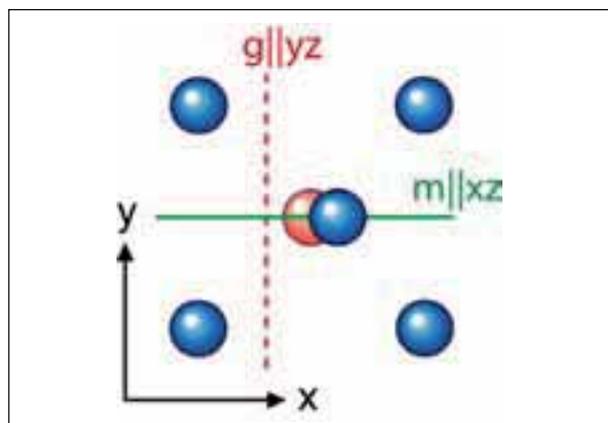


Figure 4: Sketch of the true orthorhombic atomic positions (blue balls). If the system were tetragonal the central atom would be at the red position. The mirror (green) and glide-mirror (red) planes are marked.

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Processing light with new technology

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The continuous expansion of the global communication network in the past decades has been relying on opto-electronic devices based on so-called direct-gap semiconductors such as gallium arsenide. Indirect-gap materials such as silicon were obviously not suitable for optical communication. However, silicon is indisputably the material of choice for micro-electronic devices, and forms the basis of practically all consumer electronics, computers and sensors. Meanwhile, due to the obvious limitations in speed and bandwidth of purely electronic devices, the introduction of the light wave technology into the integrated circuit has been put on the top of the development list for the next decades.

Is direct-gap essential?

Semiconductor materials like gallium arsenide (GaAs) have a direct-gap; that is, the lowest electronic states in the conduction band (blue in Figure 1) are at the centre of the Brillouin zone (the Γ -point) and are vertically aligned with the highest electronic states in the valence band (or hole states). Silicon (Si) has an indirect-gap (Figure 1 left) since the lowest electronic states in the conduction band are out of the centre of the Brillouin zone. Since the transport and optical properties are normally governed by such electronic and hole states and the light-matter interaction is the strongest between the vertically aligned states, the direct-gap semiconductors like GaAs are more efficient for the applications such as lasers and light modulators. However, because of the incompatibility of GaAs

with the fabrication process, the integration of optically active devices in Si-based integrated circuits has been difficult.

Germanium shows promise

Germanium (Ge) is also an indirect-gap semiconductor but Ge might be an interesting material for opto-electronic applications: firstly, the interband transitions at the Γ -point exhibit a well-defined resonance with the transition energy, or E_0 -gap equal to 0.8 eV, which is only ~ 0.2 eV larger than the indirect-gap equal to 0.66 eV. Secondly, this E_0 -gap energy corresponds to the wavelength of 1.55 μm used in telecommunication. And finally, Ge is process-compatible with Si-based devices. However, the attempts to utilize the E_0 -gap transitions in SiGe

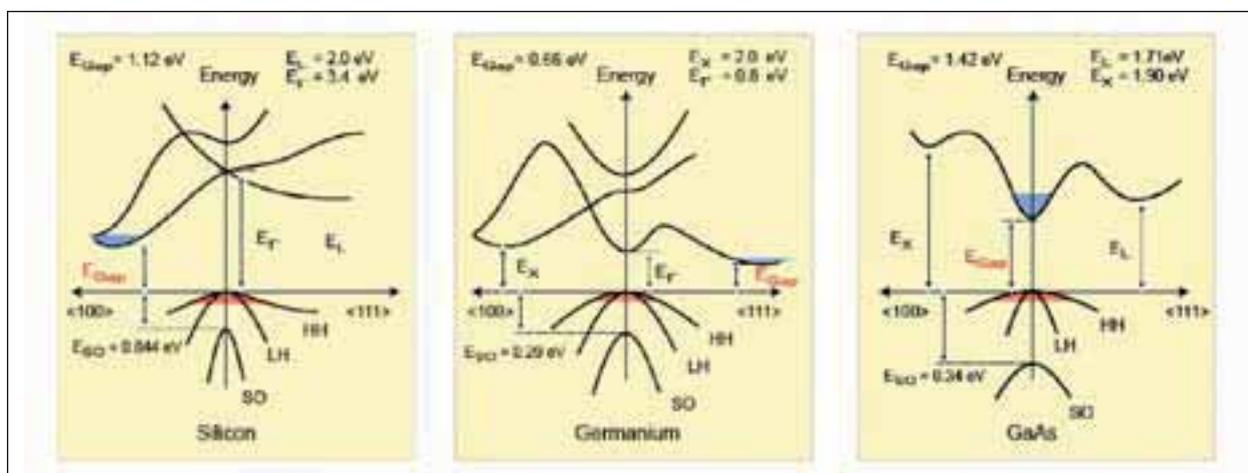


Figure 1: Band structure of silicon, germanium, and gallium arsenide (from left to right). The blue shade represents the lowest conduction band electron states, and the red shade represents the highest valence band electronic or hole states.

hetero-structures or (nearly) pure Ge islands prepared on Si substrates have not been successful so far.

In this PSI-Como collaboration, we investigated in detail the interband transition energies and absorption strength in Ge/SiGe hetero-structures on Ge-rich SiGe virtual substrates.[1] The sample consists of 10 periods of 12 nm-thick Ge quantum wells sandwiched by 24 nm-thick $\text{Si}_{0.15}\text{Ge}_{0.85}$ barriers on a $\text{Si}_{0.1}\text{Ge}_{0.9}$ relaxed buffer, Figure 2(a). The whole structure is deposited on a Si (100) substrate. The sample was prepared by low-energy plasma-enhanced chemical vapour deposition (LEPECVD).[2] This unique method is especially suitable for the epitaxial growth of SiGe hetero-structures as has been demonstrated by the record mobility of Ge quantum wells. We note that the top-most $\text{Si}_{0.1}\text{Ge}_{0.9}$ buffer layer is fully relaxed without additional annealing. This is shown by X-ray diffraction measurements of the sample in the (004) and the (224) direction Figure 2(c) shows the absorption spectrum at 17 K observed by a photocurrent measurement. A calculated absorption spectrum is also shown. A series of steps above 0.97 eV, which is ~ 0.2 eV above the indirect fundamental bandgap of Ge is ascribed to the interband absorption between quantized hole states and quantized electronic states at the Γ -edge in the Ge quantum well, Figure 2(b). Because of the steep increase of the EO-gap energy with the decrease of the Ge-content, the conduction band offset between the Ge well and the $\text{Si}_{0.15}\text{Ge}_{0.85}$ layers amounts to ~ 0.3 eV. Therefore electrons in the Ge well at the Γ -edge are quantized. This leads to an enhancement of the absorption strength. By a direct absorption experiment, we found that the coefficient of the observed interband absorption in the Ge quantum well is equal to $\sim 5000 \text{ cm}^{-1}$ and is $\sim 30\%$ larger than that of bulk Ge.

In addition, the absorption edge of such interband transition can be shifted by applying electric field perpendicular to the quantum well by the quantum-confined Stark effect (QCSE)[3]. The QCSE is one of the most important operation principles of opto-electronic devices such as light-modulators. The QCSE was demonstrated in our Ge quantum well sample in Schottky-diode geometry [1].

Conclusions

We found that the quantum confinement of the conduction band electronic states at the Γ -point leads to an efficient absorption in the telecommunication wavelength. We show that Ge/SiGe hetero-structures are optically active and applicable for micrometer size Si-based opto-electronic devices such as light-modulators and detectors, and have potential as an optical gain-medium for the telecommunication wavelength. Additionally, such efficient interband optical transitions can be exploited to inject spin-polarized carriers in Si-based materials.

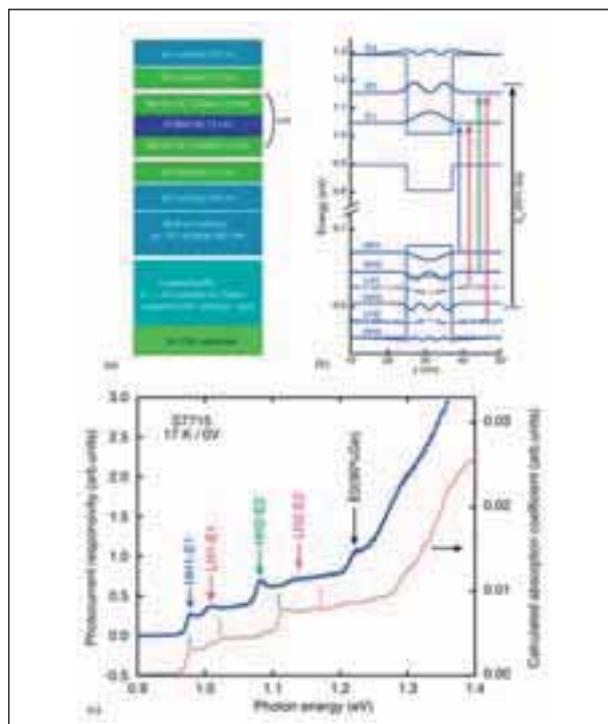


Figure 2: (a) Layer sequence of the multiple germanium quantum well sample for photocurrent and transmission measurements. (b) Band-diagram and wave functions of the electrons and holes at the Γ -point confined in the germanium quantum well. The arrows show the expected interband transitions. The dotted curve is the expected indirect conduction band edge. (c) Absorption spectrum of the direct-gap interband transitions of germanium well at 17 K. The lower trace shows the calculated spectrum.

Acknowledgements

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Superconductivity in a metalloid cluster system

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The chemical synthesis of molecular metal cluster compounds presents a bottom-up route for the generation of self-organized nanostructures composed of 3-dimensional ordered arrays of identical metal nanoparticles embedded in a dielectric matrix. Until recently, such cluster solids were always found to be electrically insulating. Lately, indications for band-type conductivity and possibly superconductivity have been reported for the crystalline ordered, giant Ga₈₄ cluster compound [1]. Such observations have now been unambiguously confirmed by very recent muon-spin spectroscopy studies performed at PSI.

Introduction and motivation

In recent years it has become apparent that the chemical route to nanostructures can be quite successful, as exemplified by the molecular metal cluster compounds. These compounds form macromolecular solids, in which the cores of the macromolecules can be seen as metal nanoparticles. Until recently, electron transfer between clusters proved negligible, resulting in materials being electrically insulating.

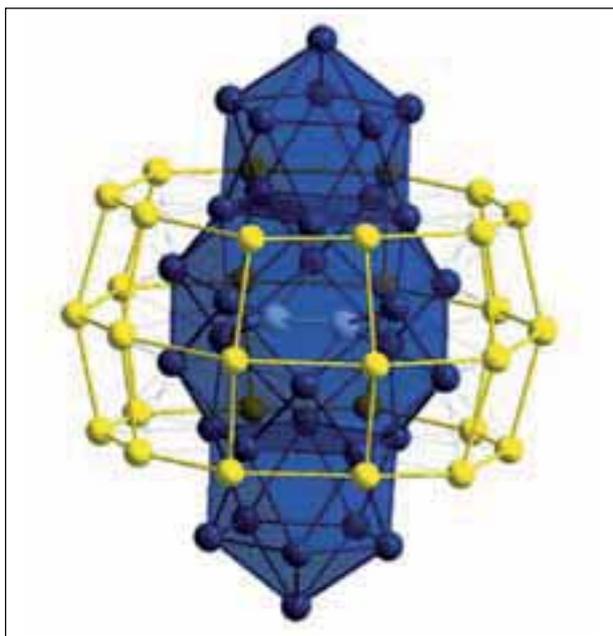


Figure 1: Representation of the 64 naked Ga atoms of the system Ga₈₄ (from Ref. [2]). A Ga₂ unit (white) is surrounded by a Ga₃₂ shell (blue) in the form of a football with icosahedral caps. These 34 atoms are surrounded by a 'belt' of 30 Ga atoms (yellow) that are also naked.

Yet the strong similarity with (super)conducting molecular crystals, such as the alkali-metal-doped fullerenes (C₆₀), suggests that, in principle, metal cluster compounds could display metallic conductivity (and even superconductivity) due to intermolecular charge transfer.

A hallmark of type II superconductivity is the occurrence of a so-called magnetic flux line lattice (FLL) created inside a superconducting sample when it is exposed to a magnetic field stronger than a material-dependent threshold. This FLL generates a well defined magnetic field distribution inside the superconductor.

Muon-spin spectroscopy (μ SR), being a local magnetic probe, is a powerful tool to measure the internal field and thereby reveal the presence of type II superconductivity. By implanting 100% spin-polarized muons in the material, the local field(s) cause a precession and/or dephasing. These effects can be measured through the detection of the positron emitted along the spin direction of the muon at the time of its decay. An additional advantage is the possibility of performing μ SR measurements in any magnetic fields arbitrarily close to zero.

The Ga₈₄ cluster system

In recent years much effort has been devoted to the synthesis of ligand-protected metal-atom clusters [2]. These metalloid systems contain some metal atoms (so-called 'naked' atoms) which do not have any contact with the ligands and which form well-defined clusters.

The main motivation for research on metalloids is to compare the structure and physical properties with those of the corresponding solid metals.

The cluster system $\text{Ga}_{84}[\text{N}(\text{SiMe}_3)_2]_{20}\text{Li}_6\text{Br}_2(\text{thf})_{20} \cdot 2$ toluene (where Me is a methyl molecule CH_3 , and thf is a tetrahydrofuran molecule $\text{C}_4\text{H}_8\text{O}$) is known as Ga_{84} . With respect to the naked metal atoms, it is the largest metalloid cluster that has ever been structurally determined (see Figure 1).

Recently evidence was provided from NMR [1] and magnetization measurements for the occurrence of band-type conductivity in crystalline ordered Ga_{84} cluster compounds, composed of arrays of giant Ga_{84} cluster molecules that display mixed-valence properties. In addition, bulk type II superconductivity was observed below a transition temperature $T_c = 7.5$ K, much higher in fact than known for bulk α -Ga metal ($T_c = 1$ K). This material was therefore thought to possibly represent a first experimental realization of a theoretical model advanced by Friedel in 1992 [3], who predicted that for a crystalline array of identical metal nanoparticles, a very weak interparticle charge transfer can still yield superconductivity with a relatively high T_c value.

It has been observed that the value of the external magnetic field required to destroy the superconducting state is – unfortunately – strongly sample dependent (B_{c2} varying from 0.3 to about 14 Tesla). Therefore, it appeared mandatory to obtain a clear and definite proof for the occurrence of bulk superconductivity, especially for samples with low values of B_{c2} .

Muon spin spectroscopy studies

We performed our experiments on the GPS spectrometer located at the $\pi\text{M}3$ beamline of the Swiss Muon Source ($\text{S}\mu\text{S}$) at the Paul Scherrer Institute, in the temperature range $2 \text{ K} < T < 10 \text{ K}$ and using magnetic fields up to 0.4 Tesla. The Ga_{84} sample (30 mg) is extremely air sensitive and required special care. It has been kept in a toluene solution with a sample/toluene mass ratio of order 80/20 to avoid loss of crystal solvent. This solution was sealed in an aluminium sample holder using an aluminium thickness of only 0.35 mm between the incident muon beam and the sample as a moderator for the muons.

Figure 2 shows the time dependence of the muon polarization $P(t)$ recorded in an external field, of 0.06 Tesla, high enough to create a FLL in the sample. A clear difference can be seen between the data measured at $T = 10 \text{ K} > T_c$ and $T = 2 \text{ K} \ll T_c$.

Above T_c , the local field is small and in agreement with that calculated based on the nuclear dipoles present in the sample. Below T_c , the stronger decay of the signal due to dephasing of the muons demonstrates the occurrence of a FLL and thereby establishes the presence of type II superconductivity.

Careful analyses of the data indicate that the full sample volume becomes superconducting. In addition, a normal state could be recovered when applying an external field higher

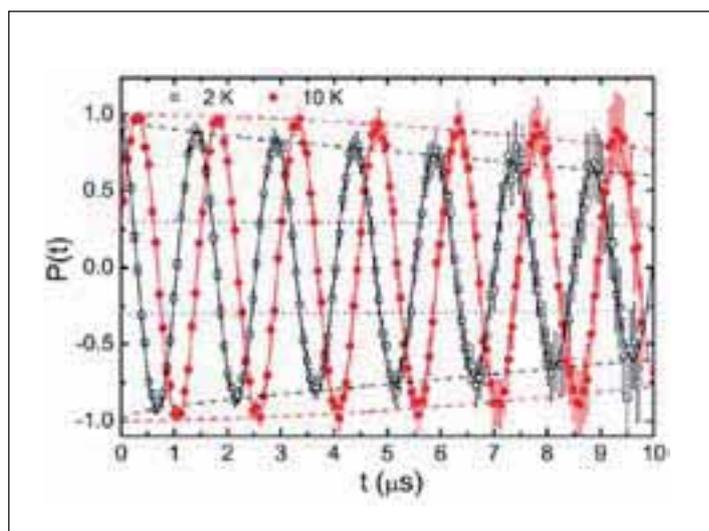


Figure 2: Polarization $P(t)$ of the muon spins, in a transverse-field experiment (field-cooling, external field of 60 mT). The data are represented in a rotating frame and, for clarity, only one of the two parts (imaginary or real) is shown for each temperature. Note the clear increase of the depolarization at low temperature.

than 0.3 Tesla, confirming the magnetization data. The temperature dependence of the depolarization rate is well described by the BCS model with s-wave symmetry.

The main results of this study, as well as a complete discussion of the mechanisms for the occurrence of superconductivity in this system, have been recently published in the journal *Physical Review Letters* [4].

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New capabilities for imaging at the cold neutron beamline ICON at SINQ

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This article reports on the latest developments in neutron imaging and presents selected examples of how users from industry and academia will be able to profit from these new possibilities in micro-tomography, energy-selective neutron imaging and phase contrast studies at the cold neutron imaging station (ICON). With these new capabilities, a major step towards covering the gap in object sizes between the capabilities of the micro-tomography beamline at SLS (TOMCAT) and the macro-scale setup at NEUTRA has been made.

Based on a very successful program on imaging of materials and components at the thermal beamline (NEUTRA facility) in sector 32 of SINQ, a second station for neutron imaging was designed and brought into operation at the end of 2005. ICON [1] receives its neutrons from the cold source at SINQ. Cold neutrons are more sensitive (less penetrating) and allow for new features and an instrument complementary to NEUTRA. During the test phase end of 2005 the higher sensitivity to material distribution determination, in particular for materials containing hydrogen was demonstrated.

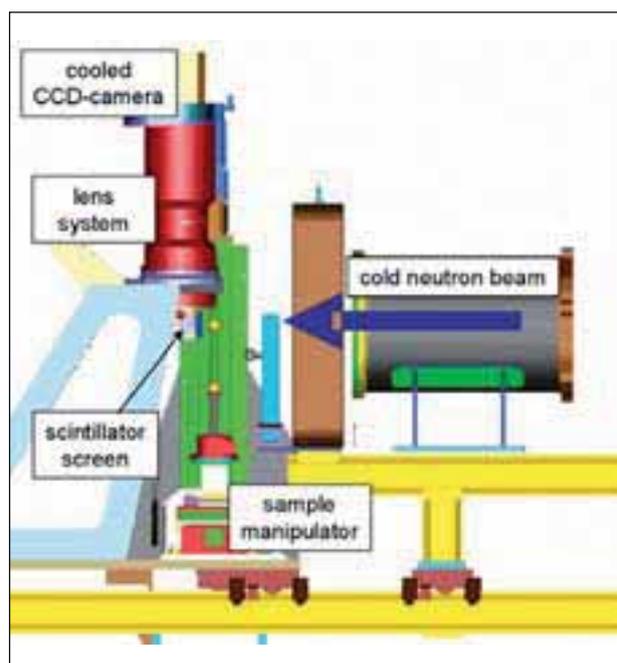


Figure 1: Setup of the micro-tomography facility at the cold neutron beamline, ICON at SINQ.

Micro-tomography at ICON

In 2006 a further step was realized with the installation of a micro-tomography setup at ICON with the aim of overcoming limitations in the spatial resolution of neutron imaging [2]. The concept is based on a new kind of scintillator screen (developed in collaboration with a Swiss company), the use of a perfect optical system, the exploitation of the high detection probability of cold neutrons, a high collimation of the neutron beam and a well-adapted CCD-camera system (Figure 1). In a first ever realization for a stationary digital neutron detector, at least 20 line-pairs per mm can now be detected in the relatively short exposure time of a matter of seconds. This is demonstrated by the image of the test pattern as shown in Figure 2, which was specifically developed together with LNM at PSI for evaluation purposes [2].

The first result with the new detector system for tomography investigations is shown in Figure 3, the nozzle of a diesel injection device. Many other research fields such as the investigation of the water distribution in electric fuel cell membranes or in the roots of growing plants will profit from this advance in detector technology.

Using a velocity selector to mono-chromatize the neutron beam i.e. to select a relatively narrow wavelength band between 2 and 7 Å, the contrast in the image depends on whether the neutron wavelength is below or above the Bragg edge for the crystal structures in the component.

First investigations of welds demonstrated that in this way texture structures can be visualised directly. This development is of particular interest for the development of dedicated imaging beamlines at future pulsed spallation sources.

The improvement in sensitivity has also been used to detect hydrogen in nuclear fuel cladding. Based on dedicated ex-

periments at quenching facilities at Forschungszentrum Karlsruhe (FZK), material changes in the cladding during and after accident conditions have been studied [3].

The determination of water distribution in running fuel cells with high resolution has also been obtained with the micro-setup. This delivered spectacular new insights into materials behaviour.

The investigation of wood properties (structure, moisture, adhesives, impregnation) from samples with relevant size (few cubic centimetres) and high spatial resolution (50 μm), is another promising area (Figure 4).

Neutrons and phase contrast

The ICON beamline was also used for a first test of phase contrast imaging neutrons. Using a setup for a grating interferometer [4], the material properties in respect to the phase-

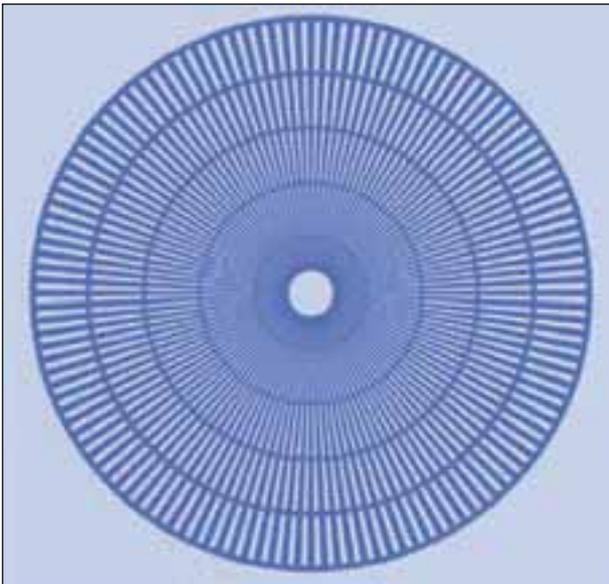


Figure 2: **Result of the test measurement with a thin scintillator screen in the micro-tomography setup (Figure 1) of a Gadolinium pattern etched at LNM. The diameter of the outer circle is only 20 mm.**

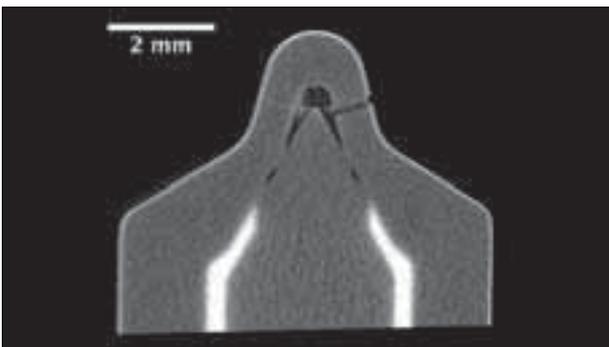


Figure 3: **Tomographic slice through the nozzle of a diesel fuel injector, where the oil (in white) was partly evaporated and the empty upper part of the nozzle could be inspected.**

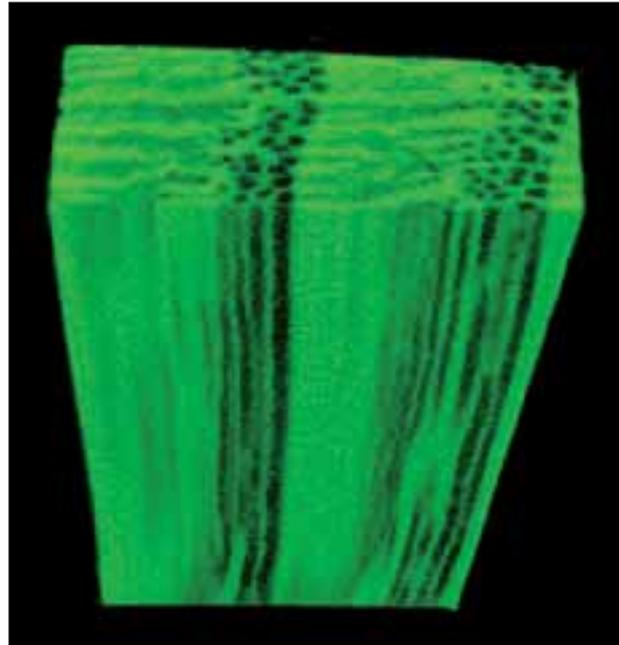


Figure 4: **Result of the tomographic inspection of a small sample of oak wood (dimensions: 5mm x 10mm x 20 mm); the annual ring structure and thin empty channels can clearly be distinguished.**

shift during neutron interaction have been directly visualized for relevant materials such as Ti, Pb, Mo and Mn. Further studies are focused onto the direct observation of magnetic domains. A permanent set-up for phase contrast imaging is underway.

There is good reason to believe that the different new options will provide a break-through in non-destructive investigations for samples of small size (up to 25 mm) requiring high resolution. With these new possibilities we will bridge the gap between the micro-tomography system at SLS (TOMCAT beamline) and the macro-scale setup at NEUTRA.

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External pressure changes molecular structure

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A major concern of chemistry and physics today is the conception of devices based upon the manipulation of the electronic, magnetic and structural properties of molecules; spin-crossover complexes and single molecule magnets being prominent amongst these. In principle, molecular deformations driven by electron-phonon interactions can also serve this purpose. In this article we demonstrate how a gross change in the molecular and electronic structure of chromium (II) compounds may be driven by a modest change in pressure.

Molecular deformations

The Jahn-Teller effect is an electron-phonon interaction manifesting in a distortion along an asymmetric vibrational mode of the molecule and a concomitant lifting of the orbital electronic degeneracy. The phenomenon continues to attract a large body of fundamental research largely due to its likely implications in the physical properties of high-TC superconductors and materials exhibiting giant magneto-resistance. The quintessential Jahn-Teller distortion results in an elongation of the axial bond lengths and a compression of the equatorial bond lengths, as illustrated for the $[\text{Cu}(\text{OH}_2)_6]^{2+}$ cation in Figure 1.

The direction of the unique distortion axis is dictated by anisotropic strain imposed by the crystal lattice. When two configurations are very close in energy, dramatic changes to the

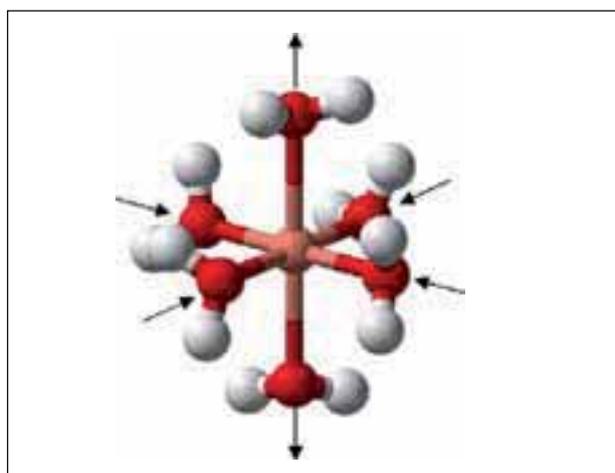


Figure 1: Jahn-Teller distortion of the copper(II) hexa aqua cation, with the long axis lying in the vertical direction.

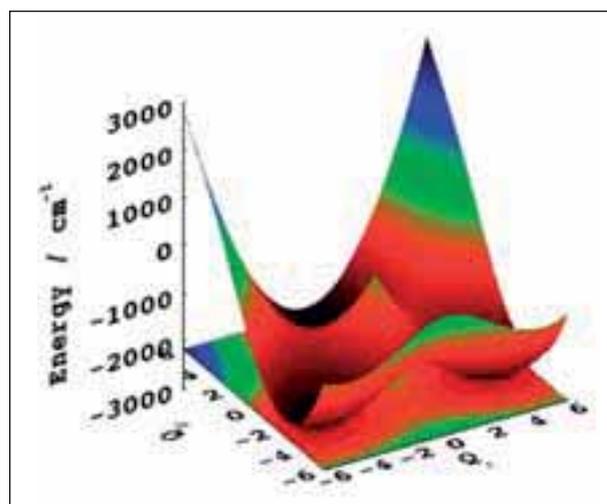


Figure 2: Surface plot of the ground state Jahn-Teller potential energy surface in cubic symmetry. The ordinate and abscissa are the Q_6 and Q_8 components of the $\nu_2(\text{CrO}_6)$ e-vibration respectively.

electronic and molecular structure of materials containing Jahn-Teller active ions can be brought about by modest external perturbations. Pioneering work on the celebrated ammonium copper Tutton salt has demonstrated that the distortion direction of the $[\text{Cu}(\text{D}_2\text{O})_6]^{2+}$ cation relative to the crystallographic axes can be manipulated by small changes in temperature and pressure.[1] Furthermore, the transition point can be tuned by the addition of impurities in the form of cations, anions and isotopic composition. One drawback of this system for practical applications is that molecular probes, such as EXAFS, are not sensitive to the distortion direction, and the change in the expectation values of the electronic co-ordinates that accompany the Jahn-Teller switch is marginal. A more promising candidate for Jahn-Telleronics is the ammonium

chromium(II) Tutton salt of formula $(\text{ND}_4)_2\text{Cr}(\text{D}_2\text{O})_6(\text{SO}_4)_2$. The $[\text{Cr}(\text{D}_2\text{O})_6]^{2+}$ cation has the $[\text{Ar}]3d^4$ electronic configuration, resulting in a 5A_g (C_i) ground term that is split to second-order by spin-orbit coupling. A Jahn-Teller switch accompanied by a significant change in the zero-field-splitting parameters, and a reorientation of the principal directions of the zero-field-splitting tensor, could be detected by the change in the magnetic moment at temperatures comparable to the zero-field-splitting.

Manipulating the potential energy surface

Elastic- and Inelastic- Neutron Diffraction studies, recently conducted here at PSI, have identified a pressure-induced switch of the long and intermediate Cr-OD₂ bond lengths. The experimental data have been modelled with a 5E_g vibronic Hamiltonian, from which potential-energy surfaces in the coordinate space of the $\nu_2(\text{CrO}_6)$ e-vibration can be constructed. These are presented in Figures 2-4. In cubic symmetry, the potential energy surface has the familiar form of a warped Mexican hat, with three potential minima. Hydrogen bonding constraints impose a low-symmetry crystal field on the $[\text{Cr}(\text{D}_2\text{O})_6]^{2+}$ cation that localises the ground state in one of the three potential wells. The data suggest that the directional nature of this low-symmetry field changes radically on increasing pressure, whilst the magnitude stays constant. Consequently, the $[\text{Cr}(\text{D}_2\text{O})_6]^{2+}$ cation is localised in different minima in the low- and high-pressure form, as shown in Figures 3 and 4. The intra-molecular reorientation of the $[\text{Cr}(\text{D}_2\text{O})_6]^{2+}$ cation is concomitant with a complete rearrangement of the hydrogen-bonding network throughout the crystal.

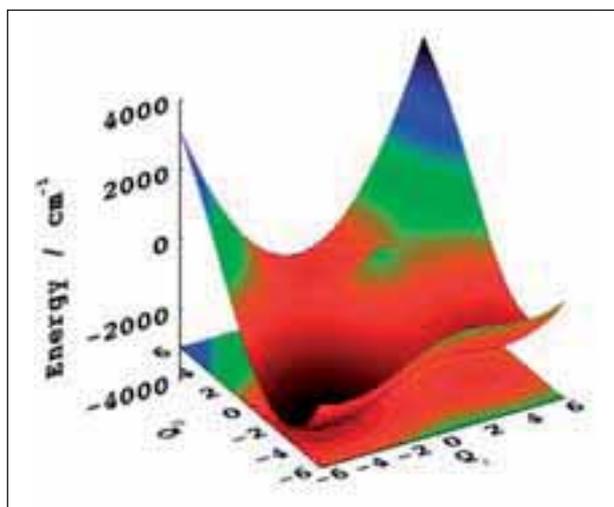


Figure 3: Surface plot of the ground E_g vibronic potential energy surface subject to anisotropic strain. The parameters are representative of $(\text{ND}_4)_2\text{Cr}(\text{D}_2\text{O})_6(\text{SO}_4)_2$ at 1 bar.

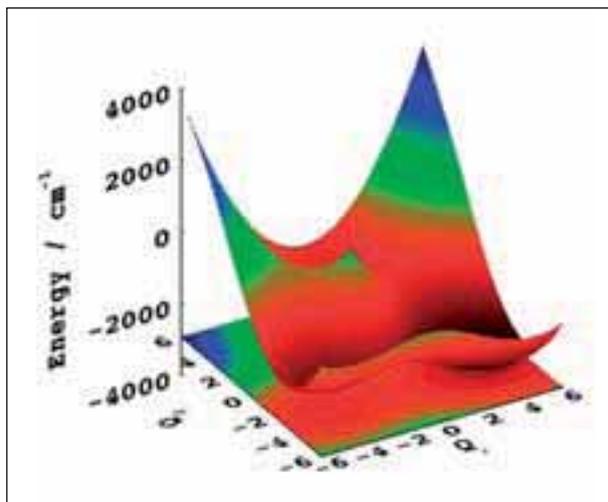


Figure 4: Surface plot of the ground E_g vibronic potential energy surface subject to anisotropic strain. The parameters are representative of $(\text{ND}_4)_2\text{Cr}(\text{D}_2\text{O})_6(\text{SO}_4)_2$ at 7.5 K bar.

Further Work

Experiments are currently in progress on zinc doped $(\text{ND}_4)_2\text{Cr}(\text{D}_2\text{O})_6(\text{SO}_4)_2$, with preliminary results suggesting that the low-symmetry crystal field can be tuned by adjusting the zinc concentration.

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Probing the structure of polymer films with neutron reflectivity

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As a consequence of their easily tuneable conductivity, conducting polymer films possess a high potential for technological applications. Of these materials polyaniline is one of the most promising, having both electronic and opto-electronic applications. In order to realise this potential, it is necessary to understand the compositional and structural changes associated with film doping/undoping. In situ neutron reflectivity can provide unique and novel insights into the spatial distributions of the polymer and solvent components within the film, providing a framework for understanding ion, solvent and polymer dynamics.

Conducting polymers find applications in electronics, optics, energy storage/conversion, (electro-) catalysis, sensors and microactuators. Their attraction lies in the possibility of combining their electronic or optical properties with both a versatility of deposition and tailoring their functionality using simple synthetic procedures. In particular, when employed as a thin film on an electrode surface, these properties can be controlled by using an applied (electrochemical) potential to manipulate the charge state (doping level) as required for the desired application.

Quite naturally, the majority of studies have focused on the electronic aspects of the doping/undoping process. However, electron exchange is merely the first in a cascade of processes that includes ion and solvent transfers between the film and its bathing electrolyte, with the polymer chain restructuring on both short and extended length scales. Our general aim is to characterize and correlate these processes with film structure and dynamics.

Polyaniline films on electrode surfaces

Polyaniline films can be deposited by oxidation of monomeric aniline in aqueous acid solution. Typically we have immersed an Au electrode in aqueous 0.1 M aniline / 1 M HClO₄ and cycled the applied potential in the range -0.2 to +0.6 V.

Upon transfer to monomer-free background electrolyte, the film redox chemistry can be characterized (Figure 1).

When the electrode is also the exciting electrode in an acoustic wave resonator, the frequency response can be used to explore the accompanying transport and dynamic processes.

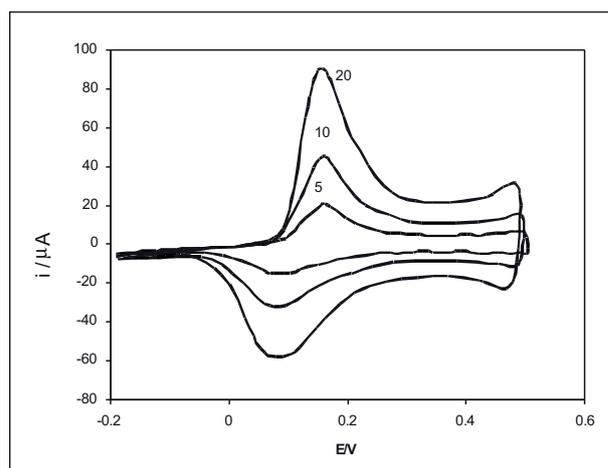


Figure 1: Voltammetric characterization of polyaniline film in 1 M HClO₄ at 5, 10 and 20 mV/s.

For the case of a thin film, resonant frequency changes respond linearly to film mass, providing a gravimetric probe of the changes in ion (dopant) and solvent populations within the film [1]. For the case of a thick film, acoustic deformation of the polymer relates to energy storage and dissipation processes, so the acoustic wave resonator is now a rheological probe. Resulting film viscoelastic properties are parameterized through the storage and loss components of the shear modulus [2]. It is also likely that the motion of the polymer chains is influenced by the presence of solvent molecules within the matrix. Thus, fundamentally, in order to account for the observed polymer dynamics (represented by the shear moduli), we need to determine the distribution and absolute ion and salvation levels in the film (not just redox-driven changes). Electrochemical quartz crystal microbalance (EQCM) data

cannot provide these. In contrast, as outlined below, we have been able to glean this information from neutron reflectivity (NR) measurements using the AMOR reflectometer at SINQ.

Electrochemical neutron reflectivity

Previously we have applied in situ NR to determine solvent and electrolyte content and profiles within polyvinylferrocene redox polymer films [3]. Using this technique, we now measured these profiles in polyaniline films as function of applied potential (i.e. different doping levels). Figure 2 shows in situ NR profiles for a polyaniline film exposed to HClO_4 solution. To determine the solvation level, the isotope sensitivity of NR measurements (contrast variation) was used and profiles collected using either H_2O or D_2O as solvent.

Fitting of the data (Figure 3) indicates that transfer from dry to aqueous environments swells the film by $\sim 25\%$ due to the incorporation of solvent and perchlorate ions associated with protonation of some of the aniline units in the polymer backbone. Interestingly, redox switching does not change the thickness or scattering length density of the film significantly. As with EQCM data [1], this suggests the dominant species moving in or out of the film to maintain electroneutrality during switching is H^+ (if only H^+ moved, the film Nb would change by $<5\%$, if ClO_4^- moved, it would change by 30%). For both reduced and partially oxidised films, the average solvent volume fraction is $\sim 20\%$, suggesting the bulk of the film to be slightly more solvated than the exposed interface. This possibly reflects a non-uniform distribution of ClO_4^- in the matrix, however further NR measurements at different HClO_4 concentrations are required to confirm this.

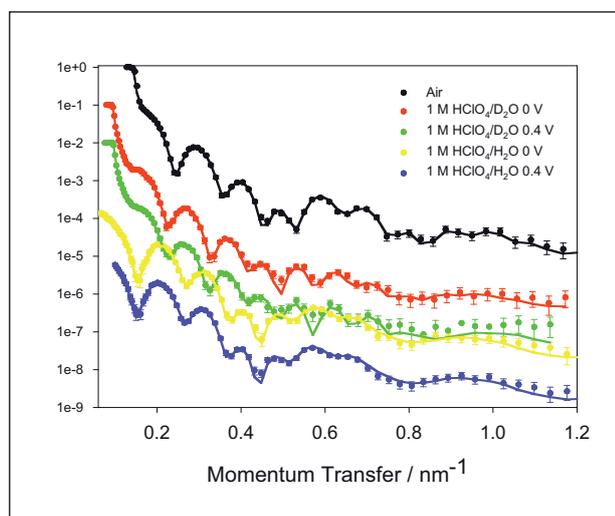


Figure 2: **Reflectivity profiles for a polyaniline film exposed to air and 1 M HClO_4 in reduced (insulating) and partially oxidized (conducting) states.**

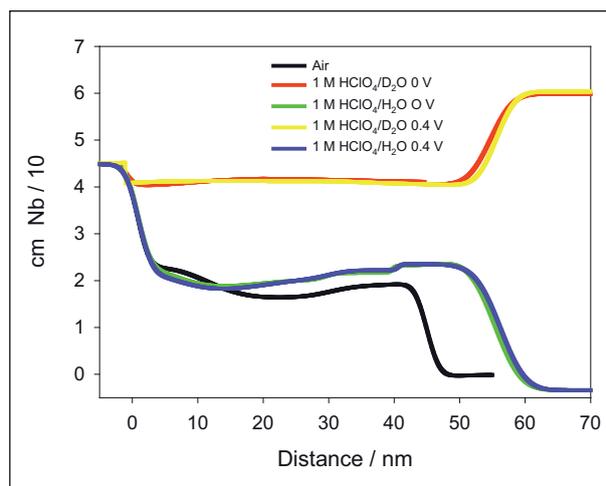


Figure 3: **Model scattering length density (Nb) profiles for polyaniline films of Figure 2. The fitting shows $\Gamma(\text{PA-NI}) = 48 \text{ nmol cm}^{-2}$, $\Gamma(\text{HClO}_4) = 21 \text{ nmol cm}^{-2}$, $\Gamma(\text{H}_2\text{O}) = 64 \text{ nmol cm}^{-2}$; redox charge passed during cycling = 14 nmol cm^{-2} .**

Future development

The acoustic wave viscoelastic data [2] indicate clear variations in shear modulus components with the electrolyte to which the film is exposed. Since this is true in both the doped and undoped states, there must be both direct effects of the dopant and indirect effects of the polymer structure, possibly solvation level or gradations in anion profile within the film. Both of these can be probed using NR and the outcomes compared with a more detailed analysis of the shear modulus signatures with electrochemical and acoustic resonator control parameters, particularly timescale [4].

The long (in electrochemical terms) data acquisition times of NR measurements – typically hours – have meant studies have generally been of films maintained under electrochemically static conditions. However, we recently developed a data acquisition procedure that allows capture of reflectivity profiles as a function of potential during potentiodynamic cycling [5]. This allows monitoring of ion and solvent fluxes for comparison with laboratory based dynamic probes such as EQCM or spectro-electrochemistry. Since many conducting polymer applications exploit rapid redox switching properties, this is an important topic for future study.

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Elucidating electronic properties by density functional theory

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Density functional theory provides a first principles approach to a wide range of properties derived from quantum mechanics of electrons for any compound. Within the accuracy provided by the inevitable approximations, it is often possible to provide support for an experimentally derived hypothesis. Sometimes such calculations lead to a contrarian view. Here the disagreement has stimulated an excellent experiment.

Introduction

Density functional theory (DFT) is an exact first principles approach to quantum mechanics that lends to a set of approximations which are useful and computationally expedient. DFT covers many types of electronic properties. This is shown for the compound highlighted here. Nitrosyl complexes show a wide variability of structure which arises as a consequence of the number of metal d- electrons available for bonding with the NO group. The nitroprusside anion $\text{Fe}(\text{CN})_5\text{NO}^-$ and nitrosyl compounds of the same class show a number of unusual properties.

For example its optical non-linearity is among the highest known; there are reversible bleaching effects; long lived metastable states can be generated by illumination with vis-

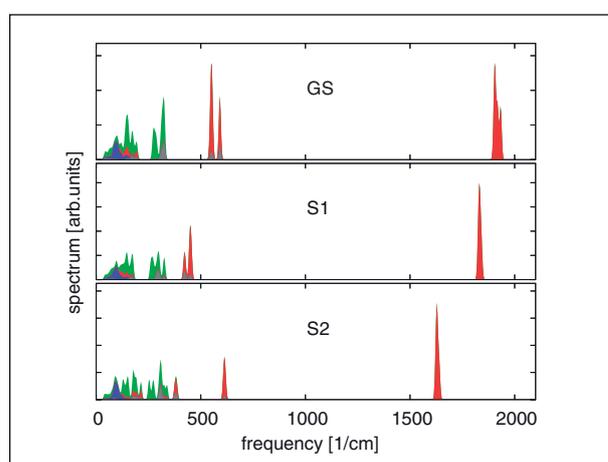


Figure 2: $\text{K}_2\text{RuCl}_5\text{NO}$ vibrational density of states: red NO, grey Ru, green Cl, blue K.

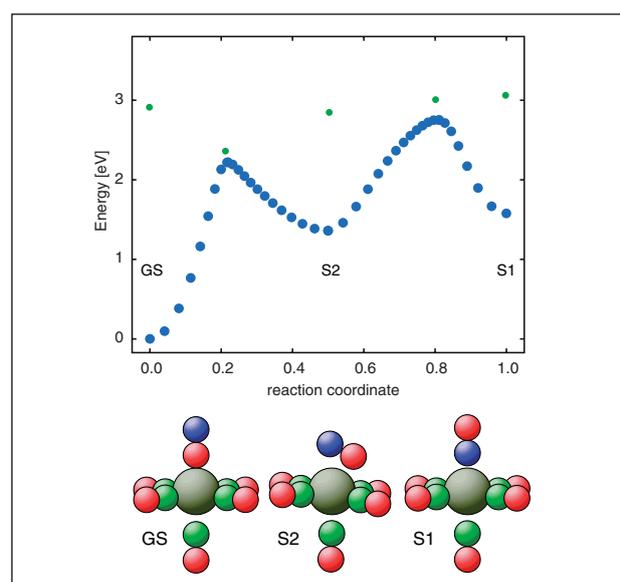


Figure 1: $\text{Na}_2\text{Fe}(\text{CN})_5\text{NO}$ energy surface along a reaction coordinate. Upper part; blue: ground state surface, green: first excited state. Lower part; grey Fe, blue O, red N, green C.

ible light; the metastable states can be clearly identified by calorimetry and can be fingerprinted by Mössbauer spectroscopy in the case of Fe compounds. Despite the multitude of possible experiments, the natures of the metastable states and the mechanisms have long been elusive. Diffraction studies in particular have shown no significant structural change from the ground state (GS). Recently, advanced photocrystallography experiments at PSI have confirmed [1] the structural predictions by DFT.

Theory and experiments

A first investigation with DFT showed [2] that the Born-Oppenheimer ground state energy surface for the nitroprusside anion has local energy minima. This theoretical finding holds true for the anion with vacuum boundary conditions, as well as in the crystalline state (SNP) with sodium counter ions and crystal water. One of the metastable states (S_1) has an in-

verted NO group. The other local energy minimum (S2) has a side-on bonded structure with rather small rotational barriers. The local minima are separated by sizeable barriers from the ground state (GS) and from each other. This is shown in Figure 1. The energy difference of the local minima above GS can be observed in a calorimeter as the heat of de-excitation. The barrier height is closely related to the observed Arrhenius behaviour of thermal de-excitation. Indeed, the calculations are in semi-quantitative agreement with observation. Furthermore, the curvature of the energy surface at the minima is closely related to vibrational spectra as observed in infrared and in optical Raman spectroscopy. The calculated spectra of GS and S1, S2 are in convincing agreement with observed spectra where the population of S1 and S2 was controlled.

This kind of comparison has been done for a number of compounds with consistent success. Figure 2 shows crystal γ point vibrational spectra for the closely related compound K_2RuCl_5NO . The softening of the NO stretch mode from GS to S1 and S2 is clearly evident. The strong splitting of the NO wag mode in the S2 state is particularly evident for this compound. Excited energy surfaces can be estimated on the basis of DFT, and are shown as well in Figure 1 as green dots. The lowest optical excitation from the ground state in SNP occurs in the visible green, and for both metastable states in the red. The excited energy surface is consistent with the observed population dynamics. The vertical excited state from ideal GS and S1 must have a Jahn-Teller instability leading to significant excited state relaxation. The relaxation allows population of S2 with green light. Similarly depopulation of S1, S2 must happen with red light in the case of the nitroprusside anion.

This population dynamics under visible light is observed and actually used to prepare non-equilibrium populations. The different optical properties of the metastable states allow the convenient monitoring presence and concentration of S1 and S2.

The changes in electron density can be fingerprinted via the Mössbauer quadrupole splitting in the case of Fe complexes. The calculated quadrupole splittings are in very convincing agreement with observed spectra.

Mössbauer spectra offer an independent way of monitoring the population of S1 and S2. Indeed the metastable states were discovered originally via the Mössbauer spectrum.

Direct observation

Despite the coherence of DFT with above experimental findings, a direct observation of S1, S2 by diffraction methods remained with mixed success [3] or even seemed to contradict the theoretically supported hypothesis [4]. Yet no alternate hypothesis could be forwarded, that would be in reasonable accord with other than diffraction experiments. It is clear that

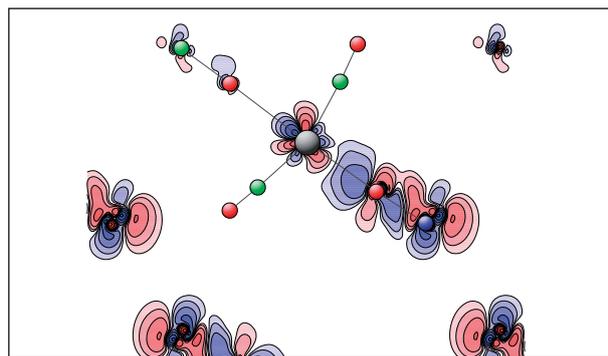


Figure 3: **Difference of deformation density between metastable state S1 and GS in mirror plane of crystal, contours 0.05, 0.11, 0.24, 0.5 ...e/Å³.**

a crystallographic observation of a population of metastable states is quite a challenge. In very well controlled experiments [1] positive evidence for the predicted structures was finally found by neutron diffraction [5]. With X-ray diffraction it should in principle be possible to observe details of the electron density. Figure 3 shows a calculated map of the difference of S1 and GS deformation density in the symmetry plane of SNP. Based on the experience with the successful neutron experiments, a new attempt for such an X-ray diffraction measurement will be made in 2007.

Conclusion

This theme has led to a constructive and stimulating interplay between a number of different experiments and theories. At PSI, such investigations have helped to identify point defects in bulk crystals and link with the soft X-ray near edge absorption fine structure as fingerprints. A special point defect is the muon, which has been addressed in a previous project. Another area of study concerns the structure and properties of surfaces and interfaces; projects here are ongoing. Also under investigation is the magnetic structure of bulk and molecular compounds, a recently published study addresses magnetic metastability in magnetic semiconductors. In addition, microscopic understanding of surface chemistry is aided by DFT.

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In-situ mechanical testing: neutrons, X-rays and simulations

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PSI's neutron source and its light source offer particularly interesting opportunities to investigate in-situ structural and mechanical behaviour of materials. A research programme has been implemented to investigate size effects in plasticity resulting from confinement of internal and external length scales. Experiments are being developed at the Pulse Overlap time-of-flight Diffractometer (POLDI) of SINQ, the materials science beamline MS4 and the micro-focus beamline MicroXAS of the SLS. Experimental research is being accompanied by large scale computational modelling.

Microstructure and mechanical behaviour

Whether a metal-based component is designed for use in an airplane or whether it will be integrated in a micro-electro-mechanical system (MEMS), the microstructure and shape of the object will determine its mechanical performance. The desire to develop materials where strength and functionality are combined has driven materials research into two types of miniaturizations: confinement of microstructural length scales to the nanometer scale and confinement of object dimensions to the micron- and even sub-micron scale where the actual size is predominantly determined by functionality. Examples of the first type of miniaturization are nanocrystalline and nanocomposite metals and multilayered or single layered coatings. Free standing sub-micron wires and beams used in sensors and actuators are typical examples of the second type of miniaturization. It has been demonstrated that the mechanical behaviour is strongly length scale dependent and that deformation properties cannot be understood by simply extrapolating our knowledge from conventional plasticity laws. There is a strong need to understand size-dependent plasticity in order to develop new predictive models. This research area exploits synergies between computer simulations and experimental research, where the latter benefits from in-situ testing techniques following the dynamics of microstructures during deformation [1]. PSI's research group Materials Science and Simulation (mss.web.psi.ch) has, with the help of beam scientists of the time-of-flight strain scanner POLDI at SINQ and the two beamlines MS4 and MicroXAS at SLS implemented three in-situ mechanical testing techniques to study the dynamics of length scale dependent deformation mechanisms.

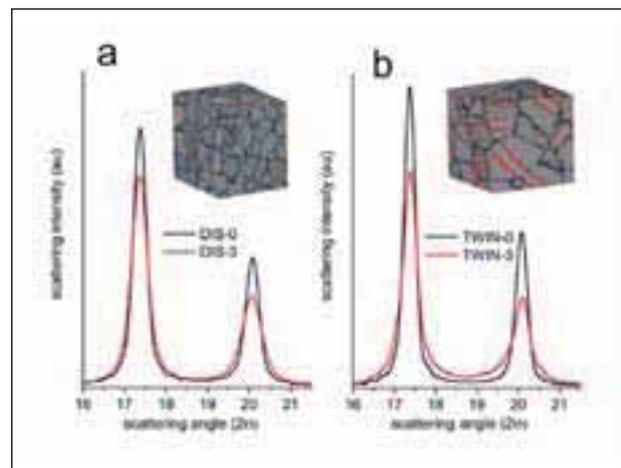


Figure 1: **Calculated diffraction pattern from MD simulated samples with (a) dislocation and (b) twin content.**

Computational approach

Atomistic simulations involving ab initio methods and large scale molecular dynamics (MD) are performed to guide the experiments and provide input for an international multiscale modelling project NANOMESO financed within the special call between EU (FP6) and NSF (USA) [2].

One of the synergetic tools developed is the calculation of powder diffraction spectra from computational MD samples that contain a well defined microstructure with a particular dislocation and twin content (Figure 1). Because the assumptions made in conventional theories of line broadening due to the inhomogeneous stress distributions of dislocations are not valid for nano-sized grains, such an approach will contrib-

ute to the correct interpretation of experimental data measured at the SINQ and SLS.

In-situ mechanical testing

A picture of the set-up and a typical spectrum measured are given in Figure 2 for the three techniques. In-situ tensile tests at POLDI allow the study of neutron diffraction at crystallographic planes that are parallel or perpendicular to the tensile axis, providing information on transverse and axial strains [4]. This set-up is particularly interesting for the study of load-transfer in composites, as was recently done for Cu/Nb wires containing two different ‘sizes’ of Cu domains and Nb filaments [5]. Figure 3 shows the evolution of the elastic strain for individual lattice plane families versus the applied stress. The continuous increase in strain demonstrates that the Nb filaments never plastify (green curve). Peak profile analysis allows the separation of the contribution of the small and large Cu domains (red and blue curves) evidencing that the smaller Cu domains need higher loads for plastification.

In the materials beamline MS4 equipped with the special microstrip detector, in-situ tensile and compressive tests can be carried out on conventional dog-bone shape samples but also on samples with micron-sized gauge cross sections, wires or free standing sub-micron thin films. This type of experiment revealed the presence of large strains in the microplastic regime in nanocrystalline Ni, suggesting that the 0.2% yield definition is not appropriate for nanocrystalline metals [6].

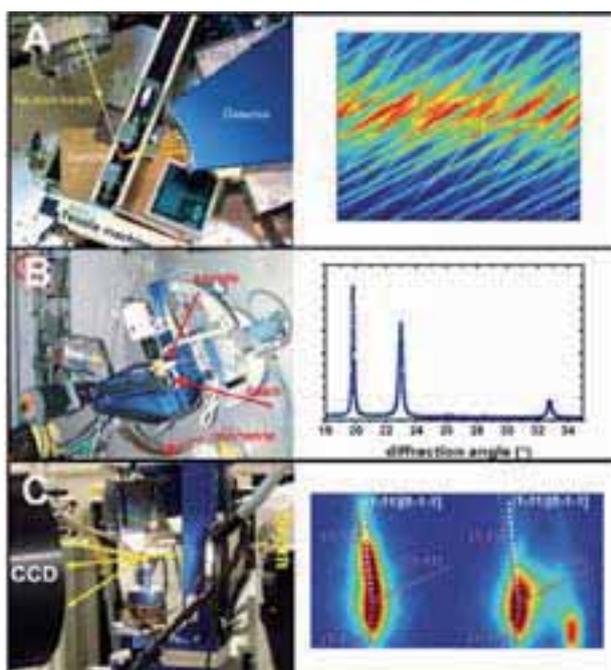


Figure 2: Typical set-up and data obtained from the three in-situ experiments: (A) POLDI, (B) MS4 and (C) MicroXAS.

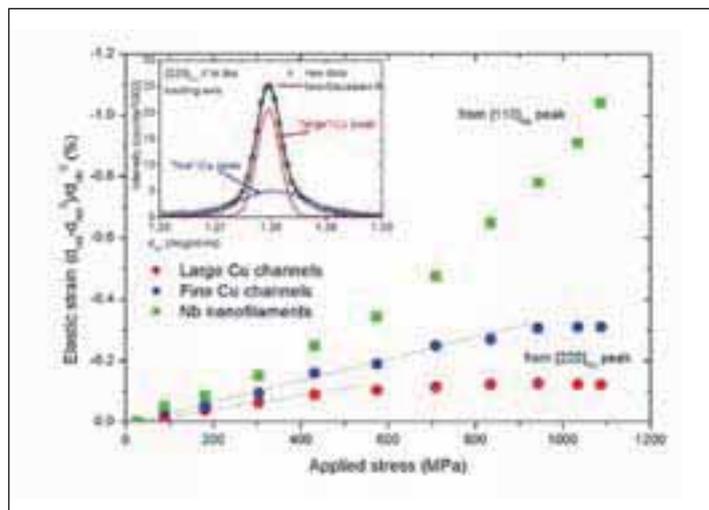


Figure 3: Stress-strain information obtained from the in-situ tensile test at POLDI for diffraction at planes perpendicular to the tensile axis [5].

The latest in-situ method developed is the real-time resolved in-situ white beam Laue diffraction micro-compression device at the MicroXAS beamline of the SLS. This set-up is especially designed for the investigation of size effects resulting from samples with confined dimensions. The experiments are conducted with a micro-compression device, equipped with a Hysitron TriboScope© single axis transducer. Static measurements revealed the presence of strain gradients in single crystalline micro-pillars [7]. Dynamical measurements demonstrate the occurrence of crystal rotation during compression, underlining the role of the pillar’s microstructure and pre-existing strain gradient.

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Higgs boson production at the LHC: supersymmetric QCD corrections to gluon fusion

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The search for Higgs bosons and supersymmetric particles will be major tasks at the forthcoming experiments at the Large Hadron Collider (LHC). For reliable analyses of the experimental data accurate theoretical calculations of the production rates are necessary. We calculated the next-to-leading order corrections to the dominant Higgs production process via gluon fusion within supersymmetric Quantumchromodynamics (QCD). We find a large increase of the cross sections and sizeable mass effects compared to previous approximate calculations.

The Higgs mechanism

The Higgs mechanism is a cornerstone of the Standard Model (SM) and its supersymmetric extensions. The introduction of the fundamental Higgs field renders the standard electroweak theory weakly interacting up to high energy scales without violating the unitarity bounds for scattering amplitudes. Due to spontaneous symmetry breaking in the Higgs sector the electroweak gauge bosons W , Z and the fermions acquire masses through the interaction with the Higgs field. Since the gauge symmetry, though hidden, is still preserved, the theory of electroweak interactions is renormalizable. In the SM one weak isospin Higgs doublet is introduced and leads to the existence of one elementary Higgs particle after electroweak symmetry breaking.

Supersymmetry

Supersymmetric extensions of the SM are strongly motivated by the idea of providing a solution of the hierarchy problem in the Higgs sector. They allow for a light Higgs particle in the context of Grand Unified Theories (GUT), in contrast with the SM, where the extrapolation to high scales requires an unsatisfactory fine-tuning of the SM parameters. Supersymmetry is symmetry between fermionic and bosonic degrees of freedom and the most general symmetry of the S-matrix. The minimal supersymmetric extension of the SM (MSSM) yields a prediction of the Weinberg angle in agreement with present experimental measurements if embedded in a supersymmetric GUT. Owing to the large top quark mass supersymmetric GUTs develop electroweak symmetry breaking at the electroweak scale dynamically. The lightest supersymmetric par-

ticle offers a proper candidate for the Cold Dark Matter content of the universe. Finally, local supersymmetry enforces gravitational interactions.

The minimal supersymmetric extension

In the MSSM two isospin Higgs doublets have to be introduced in order to preserve supersymmetry. After electroweak symmetry breaking, three of the eight degrees of freedom are absorbed by the Z and W gauge bosons, leading to the existence of five elementary Higgs particles. These consist of two neutral scalar particles h, H , one neutral pseudoscalar particle A , and two charged particles H^\pm . At leading order the MSSM Higgs sector is fixed by two independent input parameters which are usually chosen to be the pseudoscalar Higgs mass M_A and $\tan\beta=v_2/v_1$, the ratio of the vacuum expectation values of the two Higgs doublets.

Physical motivation

The dominant neutral MSSM Higgs production mechanisms for small and moderate values of $\tan\beta$ are the gluon fusion processes $gg \rightarrow h, H, A$. These are mediated by quantum fluctuations (loops), which can be calculated perturbatively. In the SM case top and bottom loops contribute, but in the MSSM also stop and sbottom loops are important for the scalar Higgs bosons h, H , if the squark masses are below about 400 GeV. The QCD corrections to the quark loops are known in the heavy quark limit as well as including the full quark mass dependence. The QCD corrections to the squark loops were only known in the heavy squark limit and the full supersymmetric QCD

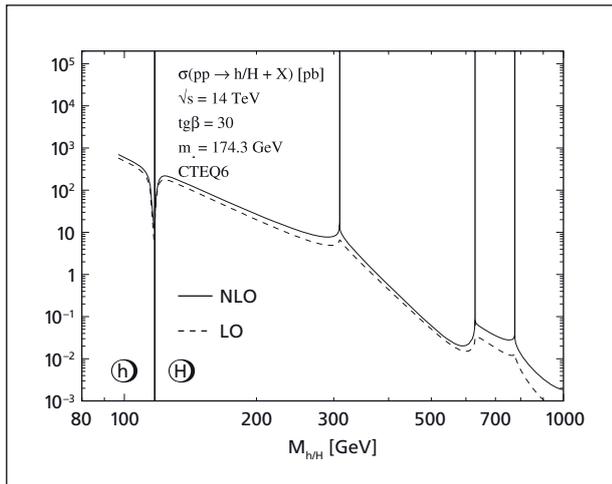


Figure 1: **Production cross sections of the scalar MSSM Higgs bosons via gluon fusion as functions of the corresponding Higgs masses for $tg\beta=30$. The full curves include the QCD corrections, while the dashed lines are the leading-order predictions.**

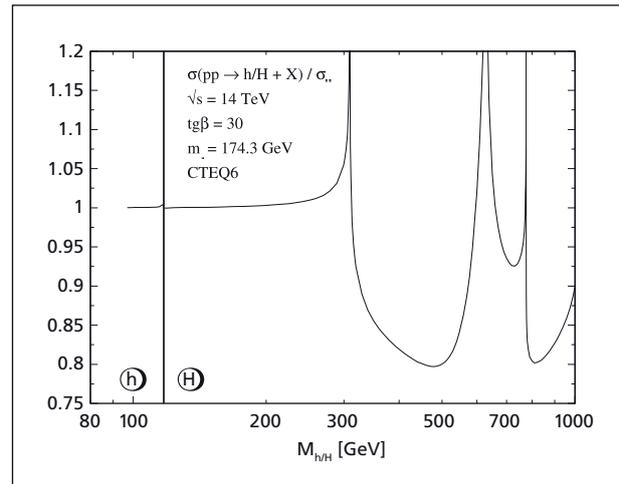


Figure 2: **Ratio of the QCD corrected production cross sections of the scalar MSSM Higgs bosons via gluon fusion including the full squark mass dependence and those in the heavy mass limit as functions of the corresponding Higgs masses for $tg\beta=30$.**

corrections in the limit of heavy squarks and gluinos. Computations of the last two contributions including the full mass dependences were missing so far. The work of Ref. [1] presents the pure two-loop QCD corrections to the squark loops including the full squark and Higgs mass dependences as a first step towards a full supersymmetric QCD calculation at next-to-leading perturbative order.

Results

The cross sections at leading and next-to-leading perturbative order are shown in Figure 1. The spikes at next-to-leading order correspond to Coulomb singularities at the corresponding squark thresholds, which will be regularized by taking into account the finite widths of the virtual squarks. This is left for future work. The QCD corrections increase the gluon fusion cross sections by 10–100%, but can be significantly larger in regions of large destructive interferences between quark and squark loops. There is a strong dependence on the (unknown) value of $tg\beta$, which is discussed in more detail in Ref. [1]. In spite of the large corrections the residual scale dependence is reduced from about 50% at leading order to $\sim 20\%$ at next-to-leading order, which indicates a significant stabilization of the theoretical predictions after including the QCD corrections. The theoretical uncertainties of our results can be estimated to less than about 20% except in the regions close to the Coulomb singularities, where the results are unreliable and require further improvements.

The squark mass effects are exemplified in Figure 2, where the ratios of the cross sections including the full mass dependence and of the approximate cross sections in the heavy squark mass limit are displayed. The squark mass effects modify the cross sections by up to about 20% and turn out to be larger than the corresponding quark mass effects. In addition they are larger than the residual theoretical uncertainties and cannot be neglected in realistic analyses. Since the gluino contributions are expected to be much smaller, the squark mass dependence obtained in Ref. [1] will be the dominant part of the differences between the heavy mass limits and a full MSSM calculation at next-to-leading perturbative order. These improved calculations will be important for the experimental search for supersymmetric Higgs bosons at the LHC and the Tevatron collider.

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The ultracold neutron source

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A new type of ultracold neutron source based on the spallation process is under construction at PSI. The essential elements of this source are a pulsed proton beam with highest intensity ($I_p > 2$ mA) and a low duty cycle (~1%), a lead spallation target, a large D_2O moderator and a solid D_2 (sD_2) converter system. Spallation neutrons are thermalized in the D_2O , further cooled in the sD_2 and, finally, some of them are down-scattered into the ultra-cold neutron range. The expected UCN density in the new source is higher than 1000 UCN/cm³, an increase of almost two orders of magnitude over the best source currently available (at ILL).

Milestones in 2006

The civil engineering work on the experimental area has been completed. Subsystems, e.g. heating, air ventilation and lighting were installed.

The installation proton beam is nearing completion: during setup, one of the beam profile monitors was damaged; the design has been slightly modified to make it more robust. A preliminary beam dump is being built in order to be able to use a test beam in summer 2007 for the commissioning of the fast (5 ms) steering system of a pulsed proton beam.

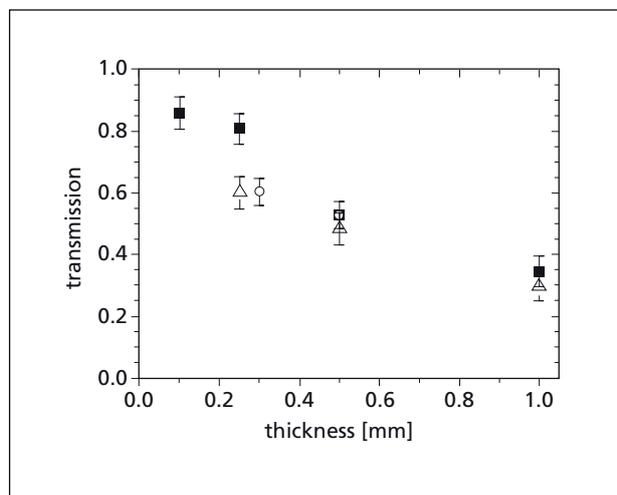


Figure 1: Transmission of slow neutrons with velocities between 5 and 9 m/s as a function of foil thickness: AlMg3 (squares), zircaloy 110 (circles) and zircaloy 125 (triangles).

The spallation target is being manufactured.

The heavy water loop is designed, several components (water storage and leakage tanks) have been ordered, all pumps, valves, filters, ion exchangers, etc. are out for tender.

The investigation of UCN losses on material walls and the measurement of the Fermi potential of diamondlike carbon and other materials were completed [1]. On the basis of these results, a prototype of a storage volume has been built and successfully tested at the ILL in Grenoble [2].

Several requirements of the federal administration (Bundesamt für Gesundheit, BAG) concerning the Safety Report have been fulfilled.

Design of the UCN source vessel

Progress has been made in the design of the solid deuterium vessel, e.g. with the investigation of materials with optimal transmission for very slow neutrons to be used for the cold moderator containment. Originally, reactor-grade zircaloy was favoured. The drawback of this material is connected with its availability in small (< 5 kg) quantities and its purity (hafnium contamination less than $5 \cdot 10^{-4}$). While at room temperature, the tensile strength of zirconium (and zircaloy) is about a factor 1.75 higher than that of AlMg₃, the factor at low temperatures is only about 1.1. That is, the foreseen wall thicknesses of the solid deuterium vessel are very similar for the two materials.

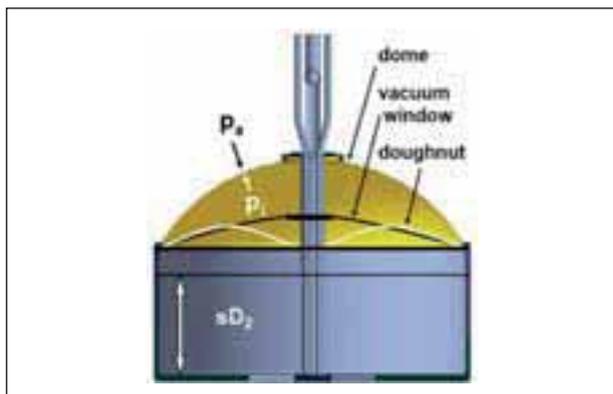


Figure 2: **Design of the cold source vessel. The vessel is a closed containment for a solid deuterium (sD_2) volume of 30 dm^3 (height $h = 15 \text{ cm}$, radius $r = 25 \text{ cm}$).**

The transmission of UCN was measured for a variety of materials, with the surprising result that aluminium alloys have a slightly better transmission compared to zircaloy, see Figure 1.

Figure 2 shows the design of the cold source vessel. In normal operation, the vessel has to withstand the following pressures:

- 1) $p_a = \text{vacuum}$, $p_i = 1000 \text{ hPa}$; this condition is during filling and freezing of the Deuterium.
- 2) $p_a = p_i = \text{vacuum}$ during UCN production.

For hydrogen safety reasons, the vessel needs to be able to withstand the following pressures at least once:

- a) $p_i = 3000 \text{ hPa}$ (at $p_a = 0 \text{ hPa}$) and
- b) $p_i = 0 \text{ hPa}$ (at $p_a = 1000 \text{ hPa}$).

These conditions could arise from a serious operational failure. The critical element is the top, which needs to be as thin as possible to reduce UCN loss. Three different versions for the top of the vessel to meet the mechanical specifications have been calculated and tested experimentally, cf. Figure 2:

- (i) a 0.5 mm thick AlMg3 ‘vacuum window’, i.e. a flat foil preformed under internal pressure of 1000 hPa ,
- (ii) an inherently stable dome of $0.5\text{--}1 \text{ mm}$ AlMg3,
- (iii) an inherently stable doughnut shape of 0.5 mm AlMg3.

The ‘vacuum window’ withstood 6 cycles under the extraordinary conditions (3000 hPa overpressure, vacuum, 3000 hPa overpressure, etc.) and broke at the 7th cycle. The dome and doughnut tops kept their respective shapes under repeated extraordinary conditions and only broke at about 8000 hPa (dome) and 6000 hPa (doughnut) overpressure. Since the transmission of UCN through thin foils is – to first order, cf. Figure 1 – reciprocally proportional to thickness, i.e. the total mass of the foil, the UCN reduction compared to a flat foil (vacuum window) is 10% for the doughnut and 31% for the dome. As a consequence, the doughnut shape has been chosen as the favoured solution for the construction of the UCN source vessel.

Neutron electric dipole moment

The most important application for the new UCN source will be to search for a finite electric dipole moment (EDM) of the neutron. This experiment is being prepared by an international collaboration from LPC Caen (F), JINR Dubna (RU), Fribur University (CH), ILL Grenoble (F), LPSC Grenoble (F), Jagellonian University Krakow (PL) and PSI (CH). Very recently also two groups from Mainz University (D) joined the collaboration.

Although the neutron EDM has been searched for with increasing sensitivity for the last 50 years, up to now only upper limits could be established.

A finite value of the EDM, if discovered, would be a sensation. It would have to be due to some new process which is not yet accounted for in the electro-weak standard model of particle physics. It would violate time-reversal symmetry at a level much stronger than observed up to now and could perhaps provide a clue for our understanding of the observed matter-antimatter asymmetry of the universe. This asymmetry needs some process which prefers regular matter over antimatter and such a process would violate CP symmetry and thereby time reversal.

Three phase experiment

The neutron EDM collaboration follows a stepwise approach in three phases: phase I, up to end of 2008, is the operation and improvement of the existing EDM spectrometer of the Sussex-RAL-ILL collaboration at the Institut Laue-Langevin (ILL), which sets the present best limit on the neutron EDM [5]. During this phase the design of a new apparatus will be performed. Phase II, 2009–2010, foresees the measurement of the neutron EDM with the improved existing apparatus moved to the new PSI UCN source. During this phase, the new apparatus will be set up and tested offline. Phase III is planned to start in 2011 and foresees the measurement of the EDM with the new apparatus for the next about 5 years until 2015. The goal is to improve the experimental sensitivity by a factor of 5 in phase II and by another factor of 10 in phase III.

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The Laboratory for Astrophysics: from instrument development to astrophysical theory

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During the past two decades, the LAP has contributed to a number of instruments on large astronomical satellite missions (RHESSI, Integral, XMM-Newton, James Webb Space Telescope). Flawless operation of missions in orbit has provided outstanding data for analysis and theoretical interpretation. The James Webb Space Telescope, successor to the Hubble Space Telescope, will carry the Mid-Infrared Instrument which promises a breakthrough in our understanding of star, planet, and galaxy formation and evolution during the next decade. The POLAR instrument will explore the magnetic field structure during the creation of black holes by measuring the polarization of the strongest explosions in the Universe, the gamma-ray bursts.

MIRI on JWST: fast progress

The James Webb Space Telescope (JWST) is the successor to the Hubble Space Telescope; it will be almost three times the size of Hubble. JWST has been designed to work best at infrared wavelengths. This will allow it to study the very distant Universe, looking for the first stars and galaxies that ever emerged, and through dust-obscured areas in star-forming regions. Compared to existing or planned observatories, JWST will have the unique advantage of combining superb image quality, a relatively large field of view and low background light with a highly stable operating environment. All these features are very important for infrared observations.

MIRI, the Mid-Infrared Instrument, is one of the four instruments on board the JWST. Built in co-operation between Europe and the US, MIRI's optics, the core of the instrument, will be provided by a consortium of 21 European institutes. MIRI will study old and distant stellar populations; regions of obscured star formation; molecular hydrogen emission from previously unthinkable distances; the physics of protostars; and the sizes of Kuiper Belt objects and faint comets. The MIRI instru-



Figure 1: The MIRI CCC.

ment will operate at 7K (−266 C), and it is very sensitive to contamination. PSI delivers, with the help of Swiss industry, the complex harness, the temperature sensors, the contamination control cover (CCC, Figure 1), and performs the long-duration test at 7K of the MIRI filter wheels.

The POLAR project

The strongest explosions in the Universe, known as gamma ray bursts (GRB), are associated with the birth of black holes. During their creation, the magnetic field structure and dynamics influence the polarization of emitted γ -rays. Thus, precise polarization detection can be a definitive tool for the determination of the true GRB emission mechanism. To obtain conclusive results, a large number of GRBs should be studied with energy and time dependence. To date, there have been no successful polarization measurements [1,2] and none of the existing γ -ray detectors on satellites (Swift, Integral, etc) have polarization capabilities [3].

PSI/LAP, together with its collaborators, is developing POLAR: a novel hard X, soft γ -ray Compton polarimeter, specially designed for measuring GRB polarization [4]. The instrument consists of an array of 1600 scintillator bars, each of them with a size of 6 x 6 x 200 mm. This design provides a wide field of view, a large modulation factor and a large active surface. The prototype is being tested in the laboratory and the demonstration model is under construction. The Chinese Space Lab and the International Space Station are candidates for the location of the experiment.

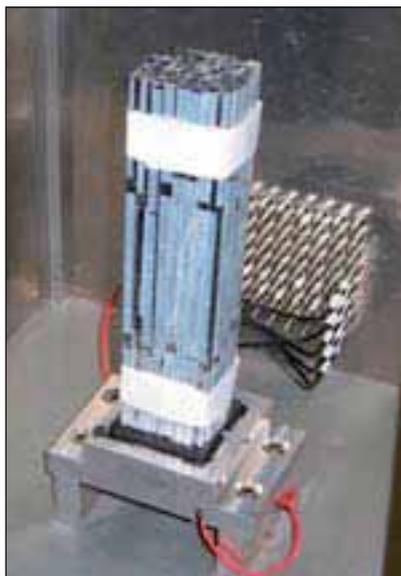


Figure 2: **Polar prototype composed of 64 scintillator bars (6x6x200 mm). The scintillator array is coupled with a H8500 Hamamatsu photomultiplier; the read-out will be performed by an ASIC from GM-IDEAS.**

Star formation: from accretion to jets

PSI/LAP has led a large international team that finished a comprehensive X-ray survey of the nearest star-forming region in the constellation of Taurus, conducted with the XMM-Newton X-ray observatory [5]. Numerous unanticipated results will require new models to be developed in the future. Accretion streams from circumstellar accretion disks seem to *cool* the otherwise hot magnetically confined coronal plasma, producing ‘soft excess’ now discovered in X-ray spectra [6]. It points to significant modifications of stellar magnetospheres by infalling gas streams. The latter seem to have been detected for the first time through excessive absorption of the coronal X-rays in very strongly accreting stars. A comparison between X-ray absorption (by gas) and optical attenuation (by dust) points to anomalous gas-to-dust ratios in these accretion streams: we interpret this as evidence for dust evaporation at some distance from the star, probably by the stellar light, and perhaps additionally by the X-rays themselves. The same stars drive massive polar outflows and jets. In their X-ray spectra, we have discovered a new, soft spectral component that may be due to shocks developing in the jets [7, 8]. This interpretation is supported by a direct X-ray image of



Figure 3: **Double X-ray jet of the accreting T Tauri star DG Tau.**

a double jet ejected from the star. These X-ray jets have been mapped out to a distance of hundreds of astronomical units (one astronomical unit is the distance between the Sun and the Earth). Notably, the jet spectrum is compatible with the soft spectral component originating from closer to the star, suggesting the same shock generation of X-ray emission very close to the star.

All results from the XMM-Newton Taurus survey will be published in fifteen different papers in a special issue/special section of the *Astronomy & Astrophysics* journal in 2007.

Numerical simulations of accretion

Hydrodynamical and magneto-hydrodynamical simulations provide an important complement to observational studies. One area in which the LAP has been active is the modelling of dust migration in protoplanetary discs. Dust tends to move towards the midplane of the disc, and also towards the star, where the density is highest. This is shown in Figure 4, taken from a smoothed particle hydrodynamics simulation using a newly developed highly parallel code. In this simulation a stellar magnetic field has the effect of evacuating the centre of the disc and preventing the accretion of gas and dust. Recent results [9] show that in this truncated disc, dust piles up in the (red) regions of maximum density. This additional mass may be sufficient to make the self-gravitating disc unstable to perturbations, and therefore to trigger planet formation.

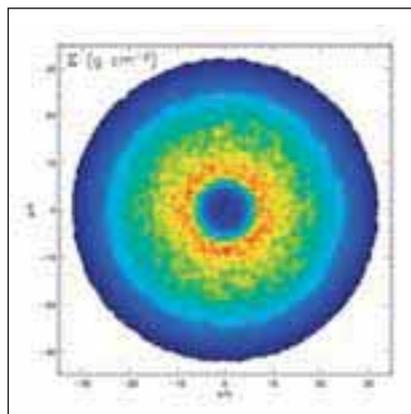


Figure 4: **Numerical simulation of a protoplanetary disc.**

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Chemical properties of element 112

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Here we present the results of an experiment aimed at the gas phase chemical investigation of element 112. The observation of two decay chains of the isotope $^{283}\text{112}$ allows a chemical property of element 112 to be quantified for the first time. The determined adsorption enthalpy on gold unambiguously discerns element 112 from noble gases and accentuates its metallic properties comparable to mercury. This experimental result also confirms for the first time the production of the superheavy elements 112, 114, and 116 in the nuclear fusion of ^{48}Ca with actinide targets as reported at the Flerov Laboratory for Nuclear Reactions (FLNR) in Dubna, Russia.

Introduction

Since 1999 the production of about 30 new isotopes of super heavy elements (SHE) up to element 118 in ^{48}Ca induced nuclear fusion reactions with actinides (see [1-6]) was reported at the FLNR. Some isotopes of the elements 112 and 114 have half-lives of several seconds allowing for their gas phase chemical investigation. There have been several attempts to investigate the isotope of element 112 with the mass number 283, that can be produced in the nuclear reaction $^{238}\text{U}(^{48}\text{Ca},3n)$ by chemical means or in purely physics experiments [7-9]. However, these experiments did not reproduce the results from FLNR (see [1-4] and references therein). The major questions of the chemical investigations [7,8] were firstly, are the chemical properties of element 112 influenced by the theoretically predicted large relativistic effects on its electronic structure, rendering it to be a closed-shell very inert non-

metal or even a noble-gas like element, comparable to radon? Secondly is element 112 behaving in a similar way to its lighter homologue in group 12 of the periodic table, mercury? Recently, the largest production cross section for the isotope $^{283}\text{112}$ was reported via the nuclear fusion reaction $^{242}\text{Pu}(^{48}\text{Ca},3n)^{287}\text{114}$ and the subsequent alpha decay of the short-lived primary product [4].

Experimental

The in-situ volatilization and on-line detection (IVO) setup connected to the cryo-on-line detector (COLD) described in [9] was used to investigate the adsorption properties of element 112 on gold simultaneously with Hg and Rn. Therefore, a stationary grid supported 1.4 mg/cm^2 ^{242}Pu target was irradiated by about $3 \cdot 10^{18}$ particles ^{48}Ca at a centre-of-target energy of 237 ± 3 MeV. The overall efficiency estimated for a Hg-like and a Rn-like species with a half-life of about 4 s were about 11% and 9%, respectively. Additional losses may have occurred due to the unknown behaviour of the primary product $^{287}\text{114}$ in the setup. The experiment was divided into two parts using two different temperature gradients in the COLD: A – 24 to -186 °C, and B: +35 to 180 °C.

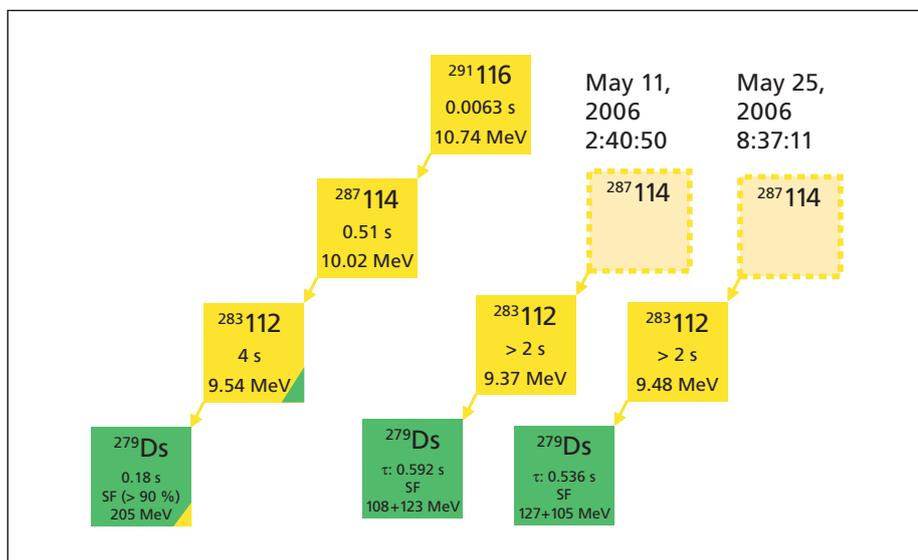


Figure 1: Comparison of the two decay chains observed in this experiment (right chains) with the decay properties of $^{291}\text{116}$, $^{287}\text{114}$, $^{283}\text{112}$, and $^{279}\text{110}$ reported by FLNR (left chain) [4].

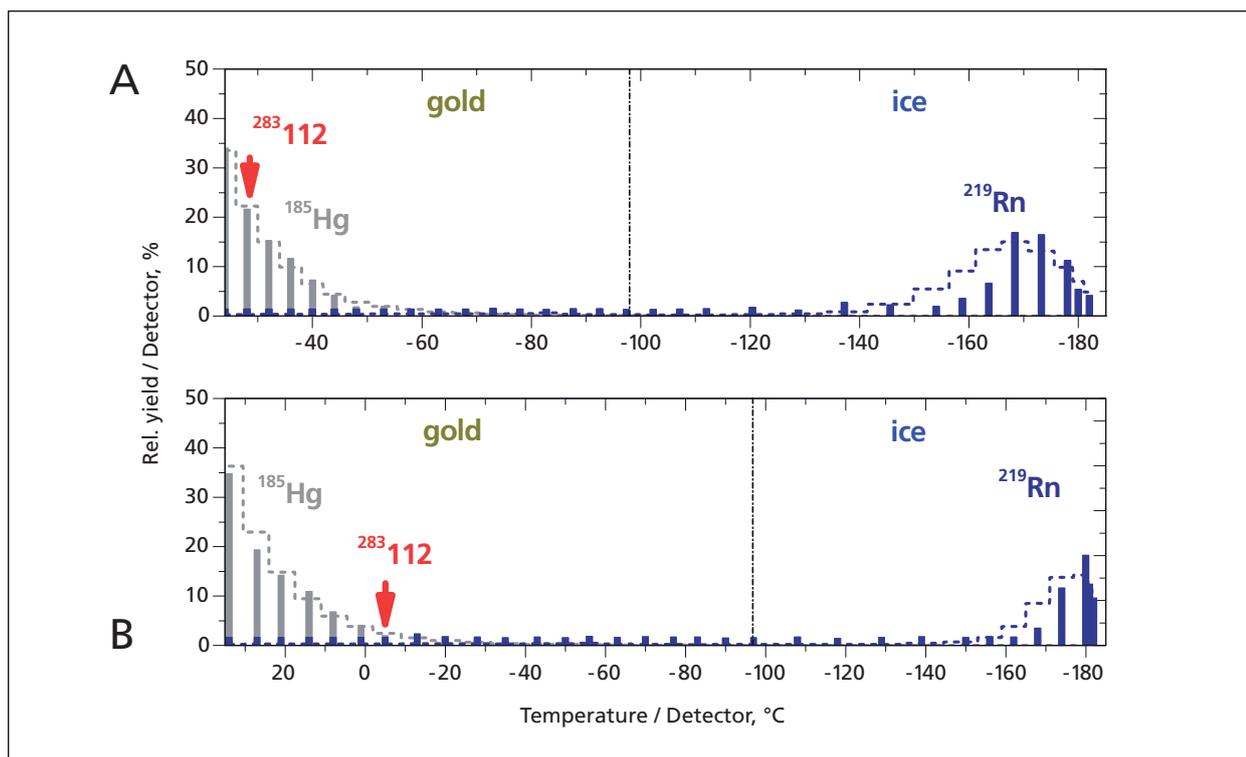


Figure 2: Thermochromatograms of ^{185}Hg , ^{219}Rn , and $^{283}112$ measured in the two applied temperature regimes A and B during the irradiation of ^{242}Pu with ^{48}Ca . The dashed lines represent the results of Monte-Carlo simulations of gas adsorption chromatography [10] with $-\Delta H_{\text{ads}}^{\text{Au}}(\text{Hg}) = 98 \text{ kJ/mol}$ and $-\Delta H_{\text{ads}}^{\text{Au}}(\text{Rn}) = 20 \text{ kJ/mol}$.

Results

During the experimental part A, for the first time in a chemistry experiment, an unambiguous decay pattern attributed to $^{283}112$ (Figure 1) was observed on detector #2 ($T = -28 \text{ }^\circ\text{C}$) in the vicinity of the Hg deposition (Figure 2, A).

Since no distinction from Hg was possible from this primary observation in the experimental part B the temperature at the inlet of the COLD was increased to $+35 \text{ }^\circ\text{C}$. Indeed, another decay chain attributed to $^{283}112$ (Figure 1) was observed on detector #7. Only 5 % of the entire Hg was able to reach this detector held at $-5 \text{ }^\circ\text{C}$ (Figure 2, B). The statistical treatment of this observation based on Monte-Carlo techniques [10] described in [8] revealed a clearly stronger interaction of element 112 with the gold surface compared to the noble gas radon and allowed for the first time to determine a chemical property of element 112, namely its adsorption enthalpy on gold surfaces $-\Delta H_{\text{ads}}^{\text{Au}}(112) = 52_{-7}^{+46} \text{ kJ/mol}$. This quantification indicates a metallic interaction of element 112 with gold, comparable to its homologue Hg. Besides this important chemical result, the confirmation of the decay properties of $^{283}112$ and $^{279}110$ anchors the nuclear charges Z of these members of the decay chains observed for the isotopes $^{287}114$ and $^{291}116$ [4] and thus bolsters the discovery of two new elements 114 and 116 at FLNR (Figure 1).

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AMS as a tool for climate research

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The Laboratory for Ion Beam Physics operates under a contract between ETH Zurich and PSI. With three tandem accelerator facilities (0.2-6 MV) the laboratory serves as a national and international centre for accelerator mass spectrometry (AMS) and for materials science. About 80 % of our efforts are devoted to AMS, an ultra-sensitive method for the detection of long-lived radionuclides; about 20 % go to materials analysis and modification. The potential of our instruments is illustrated by an example of Protactinium-231 studies.

Threefold research focus

The focus of the research programme of the Laboratory for Ion Beam Physics is firstly principle investigations of fundamental physical phenomena on which the methods and techniques of AMS and materials research are based. The relevant physics is related to ion-atom (and molecule) collisions with a focus on nuclear scattering and electronic processes (ionization, charge transfer, excitation).

Secondly, that development of high performance instruments enables us to play a leading role in the applications of ion beam techniques (see also the chapters User Facilities and Technology Transfer in this volume). In the last few years, our studies concentrated on the development of smaller, more

user-friendly and less expensive instruments. These goals have been achieved through basic research in ion beam physics, by testing new concepts and ideas, and by incorporating know-how from other fields of the natural sciences. The excellent infrastructure and know-how available allows us to design and build in-house, complete small AMS facilities.

Thirdly, the goal of our applications programme is to take part in research projects of international recognition and impact to society. Our AMS facilities can perform measurements of the major radionuclides of interest (^{10}Be , ^{14}C , ^{26}Al , ^{36}Cl , ^{41}Ca and ^{129}I , ^{236}U , $^{239,240}\text{Pu}$). Climate, and climate history, research is one of our prime research fields. We are part of more than 100 research collaborations. Most exciting are new methods exploiting the production of various radionuclides by cosmic



Figure 1: Dating of climate archives like marine corals provides access to valuable information about the Earth's climate in the past.

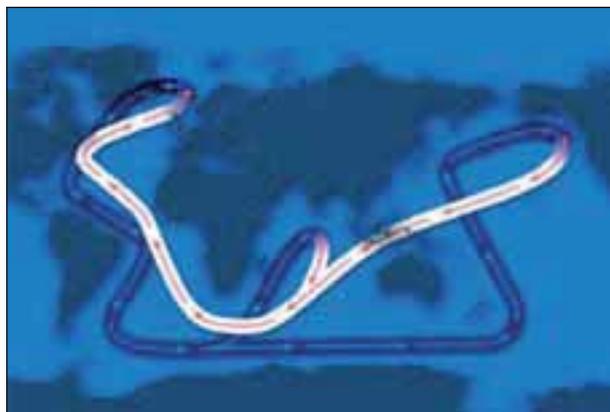


Figure 2: Reconstruction of global ocean circulation with ^{231}Pa in marine sediments.

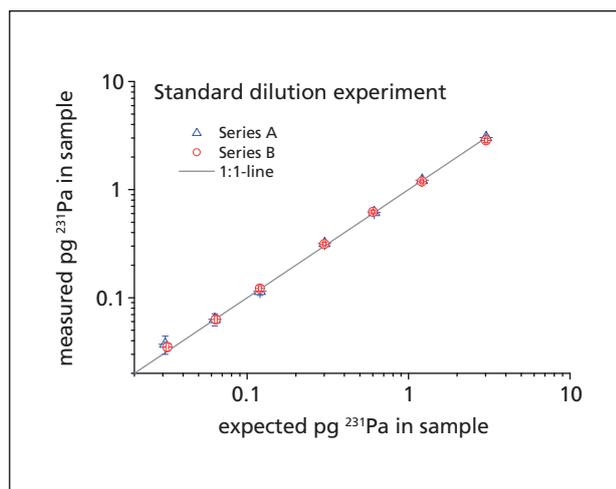


Figure 3: Standard dilution series of ^{231}Pa .

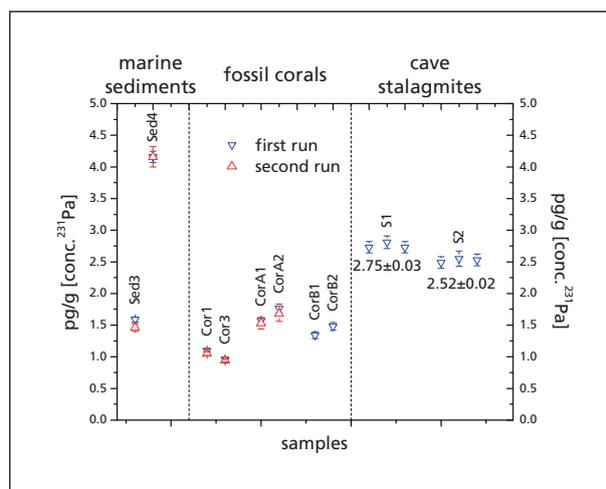


Figure 4: Measured ^{231}Pa concentration in natural samples from very different archives: marine sediments, fossil corals and cave stalagmites. The reproducibility of sample preparation and AMS measurements are shown with coral A and B samples and with the stalagmite samples S1 and S2.

radiation in rock surfaces. One method is used to date catastrophic/land-forming events and link them to major climate changes. Polar and alpine ice cores are very valuable archives of atmospheric precipitation. The records in these cores have revealed an enormous wealth of information on solar variability, geomagnetic field intensity variations, the radiocarbon cycle, and atmospheric transport of radionuclides. Other areas of our activities are archaeology, oceanography, research of extraterrestrial matter, and monitoring of anthropogenically produced radionuclides in the environment.

In this report, we illustrate the potential of our instruments by discussing pioneering experiments with a radionuclide, which has so far not been studied by AMS.

Protactinium-231, a new radionuclide for AMS

For the first time, the AMS (with the compact 0.6 MV facility TANDY) has been used to determine concentrations of the actinide Protactinium-231 ($T_{1/2} = 32,500$ yr). ^{231}Pa has two important applications in the earth sciences. First, as a part of the uranium decay chain it can be used for dating. Carbonate deposits like marine corals or cave stalagmites record valuable information about the Earth's climate system (Figure 1). Precise dating of these archives is obviously crucial for the interpretation of past climate variations and to identify the driving forces in the complex climate system. In this case, the $^{231}\text{Pa}/^{235}\text{U}$ ratio provides a totally independent clock that can be used supplementary to the widely applied $^{230}\text{Th}/^{238}\text{U}$ dating technique.

Second, ^{231}Pa is an important tracer in Paleoceanography. The $^{231}\text{Pa}/^{230}\text{Th}$ ratio recorded in marine sediments currently gives

the best estimate of ocean circulation over the last about 60,000 years (Figure 2). For example, the variation of the $^{231}\text{Pa}/^{230}\text{Th}$ ratio determined in North Atlantic Ocean sediment cores mainly reflects the variability of meridional overturning (i.e. the 'strength' of the Gulf Stream) which in turn strongly influences the Earth's climate by altering the partitioning of heat and carbon between the ocean and atmosphere.

Because naturally occurring ^{231}Pa has no very long-lived or stable isotope, an artificially produced (short lived, $T_{1/2} = 27$ days) ^{233}Pa spike is added to the samples before dissolution and chemical separation of Pa. In a first step a standard-dilution series was measured (Figure 3). The results show that with our small AMS system TANDY it is possible to determine ^{231}Pa amounts in the lower femtogram ($1 \text{ fg} = 10^{-15} \text{ g}$) range, currently limited by the laboratory blank (typically 5–30 fg). In cooperation with the University of Heidelberg (Germany), first samples from very different climate archives (marine sediments, fossil corals, and cave stalagmites) were successfully processed and measured with the TANDY (Figure 4). Our first results show that ^{231}Pa concentrations between 5 and 0.5 pg/g ($1 \text{ pg} = 10^{-12} \text{ g}$) yet can be determined with an error of about 3% (one sigma). The reproducibility of the measurements is about 1% (Figure 4: samples S1 and S2).

The above results document our ability to analyze ^{231}Pa in natural samples with a compact AMS system at sufficient precision. A proposal for a joint project with the University of Heidelberg (Paleoclimate Group) to measure profiles of $^{231}\text{Pa}/^{230}\text{Th}$ in marine sediments and to establish routine ^{231}Pa measurements with the compact AMS system TANDY was submitted. The project is expected to start in 2007.

Structural studies of ammonia channels in bacteria

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Biosynthesis of the essential amino acids requires nitrogen. Ammonium is the preferred nitrogen source for many organisms and its transport across cellular membranes is a fundamental biological process. Ammonium transport is mediated by a family of ubiquitous membrane proteins (designated Amt), found in the three kingdoms of life, whose homologues in animals are the Rhesus (Rh) proteins. We aim to understand the transport mechanism of these proteins and their functional regulation at a detailed level through structural and functional studies.

In conditions of nitrogen limitation, the uptake of the important nutrient ammonium by bacteria, fungi and plants is facilitated by a family of integral membrane proteins, the ammonium transporter (Amt) family [1]. We are investigating the mechanism of ammonia conduction by structural and functional studies. In *Escherichia coli*, the ammonia channel AmtB and the P_{II} signal transduction protein GlnK constitute a highly

regulated ammonium sensory system. Binding of GlnK to AmtB apparently inactivates the channel.

Nitrogen metabolism is tightly regulated in prokaryotes and members of the P_{II} protein family act as sensors of cellular nitrogen status. In *E. coli*, the P_{II} protein GlnK has been shown to bind to AmtB and regulate its activity in response to the nitrogen status of the cell as illustrated in Figure 1. We have been able to solve the crystal structure of this complex, which has revealed the structural basis of AmtB inactivation by GlnK [2]. The predominant view now is that Amt/Rh proteins act as channels for NH_3 (and possibly CO_2 in some cases) but not as secondary active transporters for the ion NH_4^+ as originally thought. Following the structure determination of the *E. coli* AmtB protein by us and others [3,4] we have studied a number of AmtB mutants to gain insight into the mechanistic role of two highly conserved histidine residues located in the central part of the channel.

Structure of the AmtB-GlnK complex

Crystals were obtained from detergent-solubilised, purified AmtB-GlnK complex whose formation was induced under physiological conditions through application of an ammonium shock to an *E. coli* cell culture. Data to 2.5 Å were collected at the SLS beamline XS06A and the structure could be solved using molecular replacement methods. Like AmtB, GlnK is also a homotrimer and binds to the cytoplasmic face of an AmtB trimer (Figure 1).

GlnK interacts with AmtB almost exclusively via a long surface loop (T-loop). At its tip the side chain of a conserved arginine

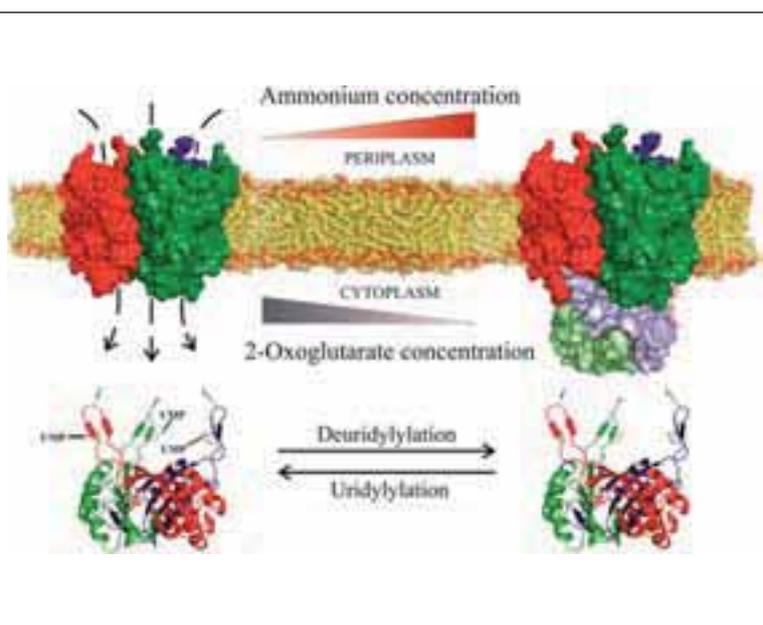


Figure 1: **Schematic diagram of the regulation of AmtB-GlnK complex formation. Uridylylation of GlnK at Tyr51 occurs under nitrogen insufficiency and prevents complex formation. High 2-oxoglutarate concentrations can dissociate the complex. AmtB and GlnK are shown in surface (top) or ribbon (for unbound GlnK) representation.**

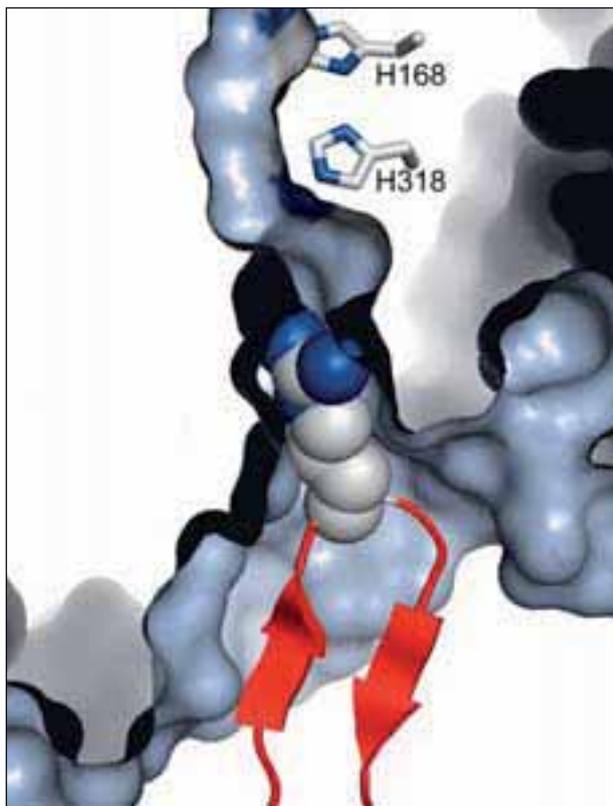


Figure 2: **GlnK blocks ammonia conduction through AmtB. Arg47 at the tip of the T-loop (red) of GlnK deeply inserts its side chain into the cytoplasmic vestibule of AmtB. The two conserved histidine residues in the pore of AmtB are indicated.**

residue (Arg47) is deeply inserted into the cytoplasmic vestibule of AmtB and blocks ammonia conduction (Figure 2). The side chain of Tyr51 is also largely buried in this vestibule explaining why uridylation of this residue prevents complex formation because of severe steric hindrance.

Mutagenesis

Almost all Amt/Rh proteins contain two conserved histidines (His168 and His318 in AmtB), which are located in the central part of the channel (Figure 2). By analyzing 14 engineered polar and non-polar variants of these histidines we show that they both are absolutely required for optimal substrate conductance (Figure 3) [5]. Crystal structures of variants confirm that substitution of the histidines does not affect the AmtB structure. In a subgroup of Amt proteins found only in fungi one of the histidines (H168) is replaced by glutamate. The equivalent variant in AmtB is indeed partially active and its structure determination shows that it can make very similar interactions in the pore and in particular fix the orientation of the second histidine side chain.

Conclusions

Structural and functional studies of the ammonia channel AmtB of *E. coli* and of its interaction with the regulatory protein GlnK have provided detailed information on its mechanism of conduction and regulation. Future work will address a number of open questions such as the mechanism of ammonium deprotonation at the pore entry. We are also interested in studying the structures of the homologous Rhesus proteins, which have a different physiological function in mammalian cells.

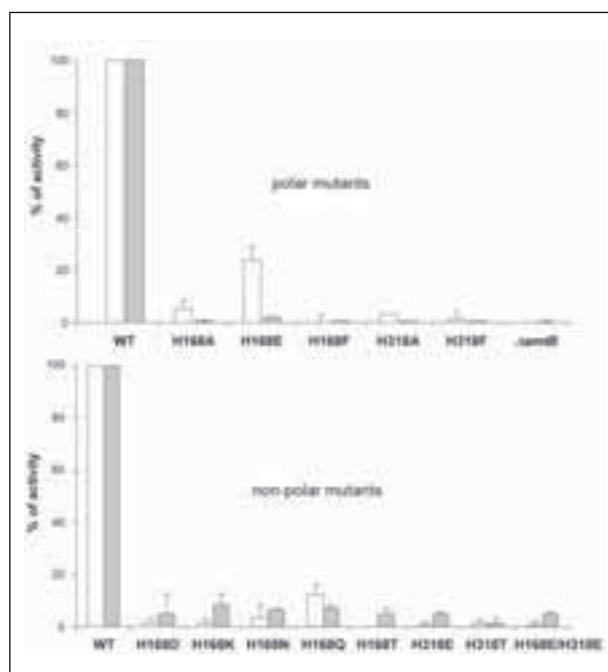


Figure 3: **Activities of AmtB variants. Mutant activities in % of wild-type (WT) activity are shown for 2 different cellular assays using ^{14}C labelled methylamine as substrate. One assay (white bars) measures initial AmtB-mediated influx, the other (shaded bars) methylglutamine accumulation [5].**

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Structure of a VEGF-VEGF receptor complex determined by electron microscopy

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Vascular endothelial growth factors (VEGFs) regulate blood and lymphatic vessel development by binding to, and thereby activating, specific cellular receptors, so-called receptor tyrosine kinases (RTK). VEGF receptors are expressed on the surface of endothelial cells, which form blood and lymphatic vessels. Here we show that in the absence of VEGF, the extracellular VEGF binding domain (ECD) of VEGF receptor 2, VEGFR-2, is unstructured. Binding of VEGF causes receptor dimerization followed by extensive changes in receptor structure. In this way, VEGF binding is communicated across the cell membrane and activates the intracellular domain of the receptor. This leads to altered cell behaviour.

Introduction

Mammalian vascular endothelial growth factors constitute a family of polypeptide growth factors, VEGF-A, -B, -C, -D and PlGF, that regulate blood and lymphatic vessel development [1]. VEGFs bind to three types of receptor tyrosine kinases, VEGFR -1, -2 and -3, that are pre-dominantly expressed on endothelial and hematopoietic cells. VEGF receptors consist of 7 extracellular immunoglobulin-like domains, a transmembrane helix, and a cytosolic kinase domain. Receptor-specific interactions have been described for PlGF and VEGF-B, which specifically bind only to VEGFR-1, while VEGF-E, a pox-virus expressed VEGF homolog, exclusively interacts with VEGFR-2. Mutation analysis of the extracellular domains of VEGFR-1 and -2 showed that the second and third immunoglobulin-like domains form the high-affinity ligand binding region for VEGF. Structural data are also available for specific VEGF ligands

and ligand receptor complexes [2-4]; however, no structural information for the entire ECD of a VEGFR has been available so far. Here we report the production of functional VEGFR ECDs and investigate the structure of these proteins by electron microscopy.

Characterization of VEGFR-2 ECD

The entire extracellular domain of VEGFRs was produced in mammalian HEK293T cells [5,6]. Two constructs were made: a monomeric protein consisting of all seven extracellular immunoglobulin-like domains, and a receptor ECD dimer held together with a GCN4 coiled coil domain. VEGF ligands were produced in *Pichia pastoris* [7]. All proteins were functional as determined by enzyme-based immunosorbent binding assays and by Biacore surface plasmon resonance analysis using immobilized receptor protein. The affinities observed for receptor-ligand interaction were 180 pM for the monomeric receptor ECD, and 56 pM for the predimerized receptor ECD.

Structure determination by electron microscopy

We next analyzed unliganded and ligand-bound receptors by rotary metal shadowing electron microscopy (Figure 1). Receptor proteins were observed as elongated highly flexible rod-like structures. No change in protein structure was observed in ligand-bound receptor molecules, indicating that this method did not preserve protein complexes.

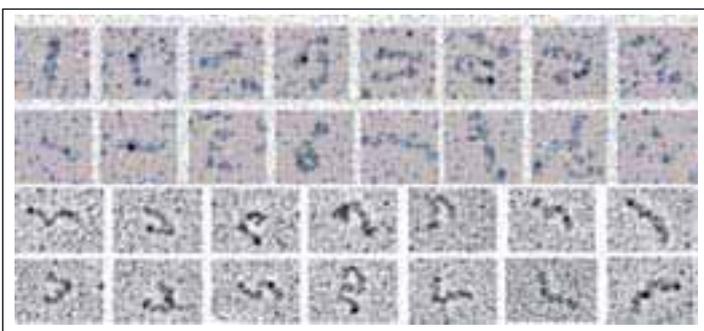


Figure 1: **VEGFR-2 ECDs analyzed by rotary metal shadowing electron microscopy. Top row monomeric VEGFR-2 ECD; second row VEGFR-2 ECD plus VEGF; third row VEGFR-2 GCN4 ECD; bottom row VEGFR-2 GCN4 ECD plus VEGF.**

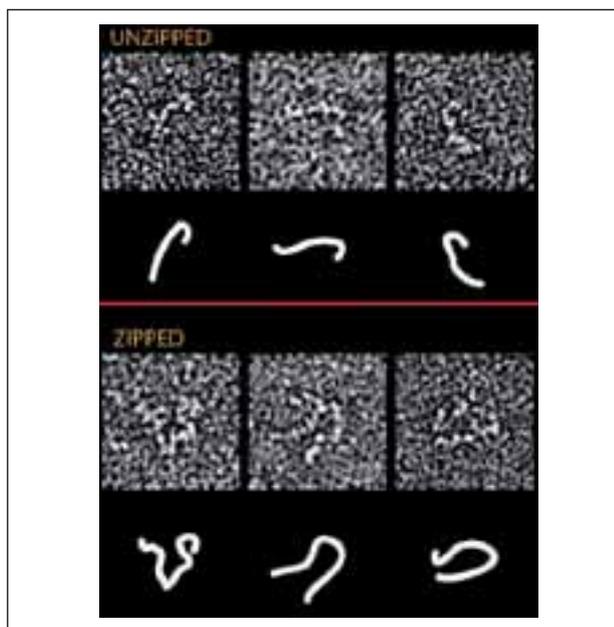


Figure 2: **Negative stain electron microscopy of monomeric (unzipped) and dimerized (zipped) VEGFR-2 ECD.**

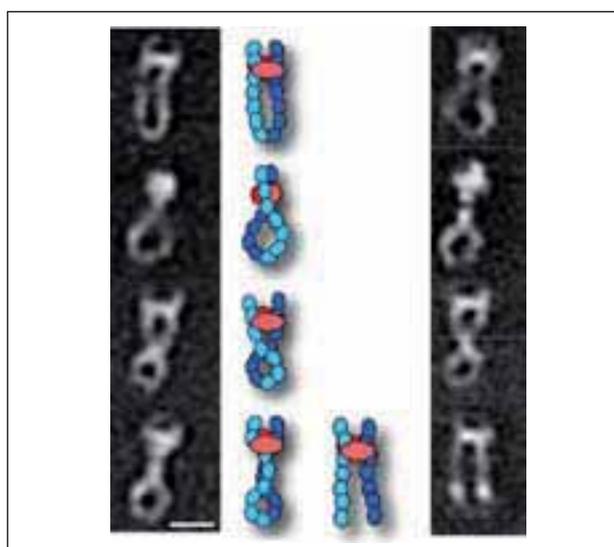


Figure 3: **Both monomeric and dimeric receptor-ligand complexes assume a rigid and well-defined structure that is held together at the ligand binding domain, immunoglobulin-like domains 2 and 3, and at the membrane-proximal domain 7. Undimerized receptor ECDs bound to ligand revealed also more flexible conformations at the membrane-proximal domain as seen in Figure 3 (bottom row on the right). Replacing immunoglobulin-like domain 7 with domain 6 of VEGFR-1 completely abolished the interaction at the membrane-proximal domain [8].**

We next analyzed VEGFR-2 ECDs by negative stain electron microscopy as shown in Figure 2. Both monomeric and dimerized VEGFR-2 ECD proteins assumed random conformations without clearly discernible tertiary structure. On the other hand, ligand-bound receptor ECDs showed a dramatic change in structure (Figure 3).

Discussion

Based on our data we propose that VEGFR-2 ECDs are highly flexible in the unbound state with no specific three-dimensional conformation. Upon VEGF binding, two VEGFR-2 ECDs come together forming multiple interactions. Membrane-distal immunoglobulin-like domains 2 and 3 are involved in ligand-mediated receptor association while the membrane-proximal immunoglobulin-like domain 7 promotes homotypic receptor interactions. Receptor dimers are further stabilized by immunoglobulin-like domain 4 through homotypic receptor interactions. In the full-length protein the resulting rigid arrangement of two receptor monomers is required for exact positioning of the intracellular kinase domains. This favors structural rearrangements of the intracellular tyrosine kinase domain that are essential for kinase activation and signaling to downstream components. Receptor-ligand complexes might be further stabilized by homotypic interactions of the membrane spanning and the intracellular kinase domains in full length receptors.

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A high throughput screening platform for structural biology

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We are building up a high throughput screening platform for cloning, expression, solubility testing, characterization, and crystallization of proteins and protein complexes. We have implemented robotics-based methods for parallel, streamlined target processing. The goal is to increase the likelihood for a given target to yield well-diffracting crystals, hence to speed up structure determination. The PSI/SLS automated pipeline ‘from gene to crystal structure’ will eventually expand to cover all steps from cloning to rapid mutant generation, biophysical and functional studies, as well as X-ray data collection.

Introduction

With recent advances in crystallography, the bottleneck for X-ray structure solution projects lies with obtaining suitable samples for crystallization. Technologies developed by structural genomics (SG) initiatives for parallel processing of thousands of targets has profoundly changed the way structural biology projects are managed. Streamlined, miniaturized, automated high throughput (HTP) protocols have become the SG standard. However, coverage takes precedence over success on individual targets. Notoriously intractable targets (membrane proteins/complexes) have only recently been added to the SG portfolio. In non-SG groups with a hypothesis-driven, small portfolio of difficult targets, the majority of project time is spent optimizing cloning, expression and purification protocols. Employing technologies and protocols adopted from SG can considerably reduce the time frame required.

The PSI BMR / SLS HTP platform

By screening a wide parameter space of target sequences, plasmids and conditions, one can determine high-yield expression conditions for most targets much faster than traditional approaches. The idiosyncratic biochemistry of such targets often demands a higher work input during the expression, purification, and stabilization stages than acceptable for an SG-type project. To combine HTP screening methodology with dedicated, in-depth characterization, we have built up a HTP technology platform encompassing a liquid handling robot for cloning and expression/solubility screening, an auto-

mated FPLC, analytical devices, a crystallization robot and a robotic crystal imager.

Target sequence, expression vector, host, and external expression condition are all screenable variables. Starting from a given cDNA, the PSI/SLS HTP platform’s task is to optimize their values and to find expression conditions suitable for mg-level production within about a month. Downstream HTP-format purification/protein characterization is used to obtain pure and stable protein for functional studies and structure solution. We subject the resulting protein samples to standard crystallization screens on a nl-drop robot. An automated imaging system records crystal growth. Hits are refined through grid screens rationally designed with dedicated software.

The SLS PX (Protein Crystallography) team builds up an automated crystallization/imaging/diffraction quality screening platform at the third PX beamline.

Our primary host is *E. coli*. Since a number of our targets require eukaryotic expression, we adapt our protocols for expression in *Pichia pastoris*, insect cells, and mammalian tissue culture cells to an HTP format. We start with the construction of a set of expression vectors for the chosen host. Only recombination-based cloning systems present the target sequence independent versatility to suit an HTP scheme. An additional requirement is the easy switch between different hosts. A comprehensive set of Gateway™ destination vectors has been constructed encoding a wide set of fusions. A generic, cleavable His₆-tag allows affinity purification and immunodetection. A major disadvantage of Gateway are the att recombination sites, which lead to incorporation of artificial amino acids. In order to create expression vectors encoding only authentic target sequence and to minimize costs, we have ported the mating assisted genetically integrated cloning

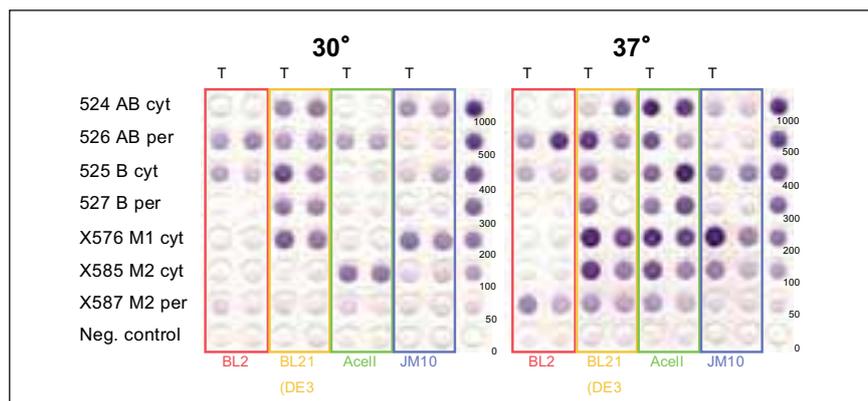


Figure 1: Dot blot showing total (T) and soluble (S) expression levels of different target proteins (left column) in microscale *E. coli* cultures grown at 30 °C (left panel) and 37 °C (right panel). Different strains are marked as coloured boxes (F. Grünwald, D. Frey, A. Prota).

(MAGIC) system by Li & Elledge [1] to our robotics platform. We screen for soluble, high-yield expression combining autoinduction media [2] with a filter binding – dot blot protocol [3] in a microscale format (Figure 1).

Preparative scale lysates are purified on an ÄKTExpress™ automated FPLC. We carry out buffer optimization screens to optimize stability against aggregation using either a Thermal Shift Assay [4], or an Optimum Solubility Screen [5].

Initial crystallization screens are performed on a Phoenix nl-drop dispensing robot. It sets up a 96-well plate in <3 minutes. Crystal growth is monitored on a RockImager™ imaging robot. Refinement screens designed with RockMaker software are run on the Phoenix.

The fully automated robotics crystallization, imaging, and plate mounting facility setup under construction at the SLS third protein crystallography beamline will allow the screening for diffraction quality directly in the drops.

First results

Several projects have already been carried out or initiated on our HTP platform. The first centers on enzymes processing *micro*-RNAs [6]. ~80 target variants (domains/domain combinations) have led to the construction of ~300 expression clones, ~50 of which led to soluble expression. About 20 of these could be produced at large scale, a figure that is about to rise with protocol optimization. Several targets have proceeded to the crystallization stage (Figure 2).

For one domain, high resolution diffraction data have been collected. Another platform-based project deals with Neuropilin, a mediator for angiogenesis, cell adhesion, and axon guidance. Several more HTP-based projects have reached the cloning stage or are on the drawing board.

The BMR/SLS HTP technology platform covers the entire ‘structure solution pipeline’. Validation with real projects has demonstrated the power of this approach. The next goals are to streamline the processes further, and to implement a laboratory information management system. A LIMS will be crucial

to document the entire platform work and sample flow, and serve as a diagnostic tool allowing data mining for continuous further optimization of protocols based on target class- and protocol-specific experiences.



Figure 2: Crystals of a domain stemming from an *Arabidopsis* miRNA processing enzyme. They diffract to 1.7 Å resolution.

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Advances in biomedical and medical X-ray imaging

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Based on the recent invention of a method for X-ray phase-contrast radiography [1], we developed a novel, high-sensitivity phase-contrast tomography scheme for biomedical and medical applications. Here we report on how the method can be used to obtain *in-vitro* tomographic images of biomedical specimens with unprecedented quality and resolution, without use of contrast agents. The results are potentially interesting from a clinical point of view, since a similar approach can be implemented with standard X-ray generators, as currently used in the medical and clinical environment.

X-ray computed tomography (CT) is an invaluable three-dimensional medical imaging method. The technique yields excellent results where highly absorbing structures are embedded in a matrix of relatively weakly absorbing material (like bones and tissue in the human body). If, however, the differentiation of weakly absorbing materials, e.g., pathologies in the soft-tissue structure, is the subject of interest, then the contrast achieved by the currently existing, absorption-based X-ray methods is limited, unless contrast agents are used. Phase-sensitive imaging can overcome these limitations and yield good contrast for soft-tissue structures. Phase-contrast imaging relies on refraction, or changes in the angular trajectory of X-rays. Just as light rays bend when they enter water from air, X-rays deflect as they travel through objects of varying densities. As reported previously [1-3], this effect can be measured using a grating interferometer and detailed radiographic phase-contrast X-ray images can be obtained. To extend this two-dimensional *radiographic* approach to three-dimensional *tomographic* imaging, the specimen is rotated around an axis perpendicular to the X-ray beam and several hundred projections are recorded. Using adapted filtered back-projection algorithms, a three-dimensional volume data set of the specimen can be reconstructed in the computer [3-6].

Improved contrast for biomedical X-ray CT

To evaluate the potential impact of this novel phase-contrast computed tomography method for high resolution and high sensitivity biomedical imaging applications, we carried out

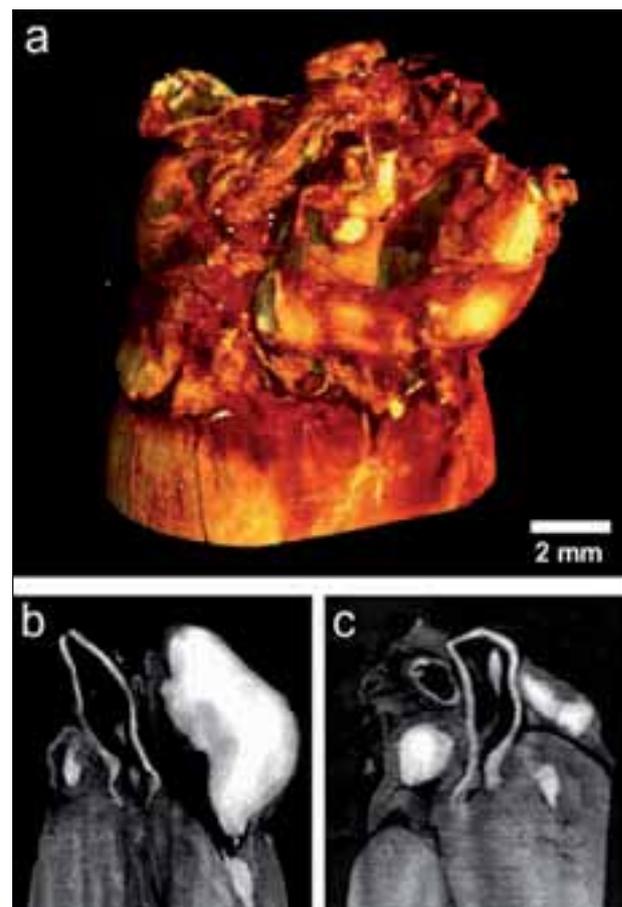


Figure 1: *In-vitro* X-ray phase-contrast tomography synchrotron results obtained on a rat heart fixed in formalin.

a, Three-dimensional rendering of the reconstructed volume data set.

b,c, Frontal and sagittal tomographic slices reveal structural details, without use of contrast agents. (Data measured in collaboration with P. Cloetens, ESRF, Grenoble.)

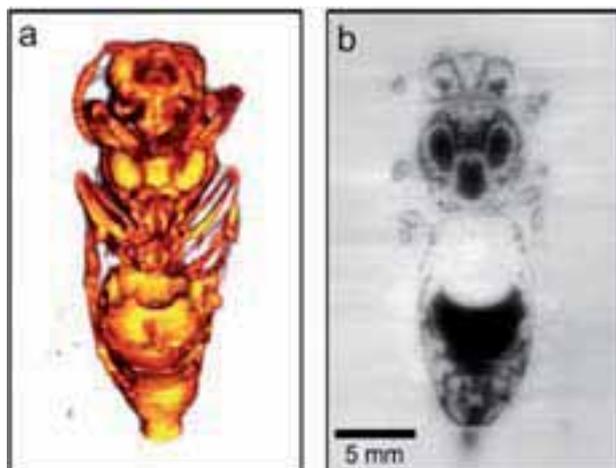


Figure 2: **Post-mortem phase-contrast X-ray CT results obtained on a large insect (a hornet) using a standard X-ray tube source.**
a, Three-dimensional rendering of the reconstructed volume data set.
b, Tomographic slice (see [7] for more details).

numerous *in-vitro* synchrotron experiments on biological specimens.

Figure 1 shows results for one example, a rat heart fixed in formalin solution. Although usually difficult to achieve based on X-ray absorption CT scans, our phase contrast CT method clearly resolves the different tissue components, i.e., the fatty tissue matrix and the heart muscle structure. Moreover, details of the blood vessel network in the heart are clearly visible. Importantly, these results were obtained without use of contrast agents, which are usually required in absorption-based X-ray CT methods.

Based on these *in-vitro* results, we envision that *in-vivo* applications are feasible in the near future, after further optimization of the method.

Towards medical applications

While this unique phase-contrast X-ray CT method is now available as a standard user option for high sensitivity biomedical investigations at the TOMCAT beamline of the SLS, we have further explored its potential for medical and clinical applications.

Clearly, clinical applications require the use of standard and commercially available X-ray generators, since it is not feasible to implement highly brilliant synchrotron sources in a clinical environment or transport all patients to a synchrotron site. In that respect, the experience gained from phase-contrast X-ray CT experiments at the SLS turned out to be crucially important to optimize and further develop the method, until it finally could successfully be transferred to standard X-ray generators [7].

Figure 2 shows first examples of the successful implementation of phase-contrast CT at a standard lab-based X-ray generator. The specimen used was a large insect (hornet). In particular the tomographic slice through the reconstructed volume data set reveals details of the internal structure of the sample (Figure 2b).

The results further illustrate that our method provides an alternative approach for performing X-ray CT scans without the explicit necessity of absorbing X-rays in the object. This is because the phase-contrast signal, which we use to perform the X-ray CT reconstruction, relies on refraction and not on absorption. A further development of the method toward higher X-ray energies, and correspondingly lower absorption, thus potentially provides a significant dose reduction.

These first proof-of-principle results open the way for future medical applications of phase-contrast X-ray CT. Through collaborations with industrial partners, the method will further be developed and may finally yield significant improvements in the soft-tissue sensitivity of medical X-ray imaging applications in a clinical environment.

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Bacterial surface layers studied by neutron reflectometry

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The study of bacterial surface layers (S-layers) stability under extreme solvent and temperature conditions is a very important aspect of biomimetic surface building. The influence of the temperature on the structure of recrystallized bacterial surface layers (S-layers) on polyelectrolyte multilayers has been investigated for the SbpA protein from *Bacillus sphaericus* CCM2177. From atomic force microscopy (AFM) investigations it is known that S-layer loses its two-dimensional crystalline structure at 55°C. Neutron reflectometry (NR) measurements showed that the S-layer thickness decreases at 55°C. The loss of the nanostructure is irreversible when this is caused by thermal treatment.

Crystalline bacterial cell surface layers (S-layers) are composed of a single protein or glycoprotein. Isolated S-layer subunits are able to assemble into (mono) molecular arrays on lipid films, liposomes and solid supports, making them an important tool for biophysical and technological studies [1].

S-layers representing the outermost barrier of most bacterial cells contribute to their protection and these proteins normally display an unusual physical and chemical stability. An important biological issue regarding the S-layers is their

stability under extreme solvent and temperature conditions. Thermal denaturation studies show that recrystallized S-protein layers on i) hydrophilic silicon wafers, and ii) secondary cell wall polymer (SCWP), the natural cushion for the protein layer in bacteria, loses the 2-D crystalline structure at 70 °C, this being an irreversible process [2].

AFM is a powerful tool to investigate the topography of bio- and non-biomaterials [3]. NR complements AFM method by providing information at vertical dimension. NR, with its abil-

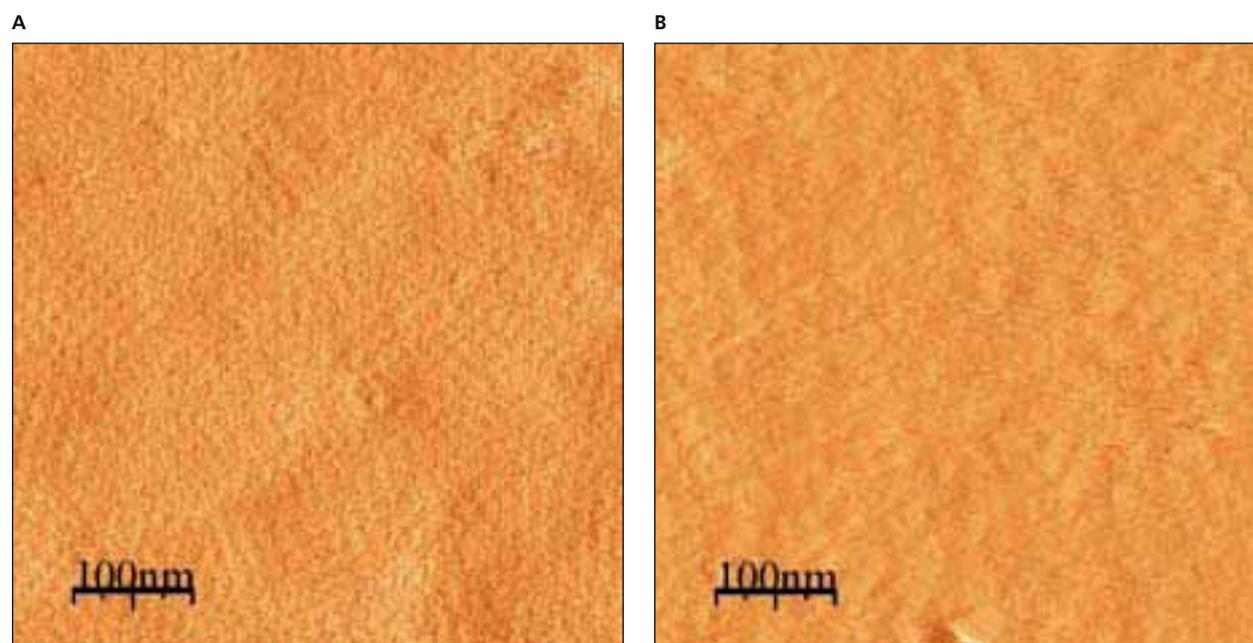


Figure 1: AFM deflection images measured at room temperature in 100 mM NaCl aqueous solution. (A) S-layer as was formed on Si/PEI(PSS/PAH)₂/PSS and (B) after 10 minutes exposure at 55°C.

ity to study the changes in the density of the S-layer as a function of the temperature, the film thickness and scattering length density (SLD) at the solid/liquid interface, is a suitable tool to follow the changes in S-layer structures with the temperature.

Previous neutron reflectometry (NR) experiments showed the capability of the method to supply information about the structure of the S-protein layers. The thickness, SLD and the roughness of S-layers at solid/liquid interfaces were obtained [3].

Course of experiments

We studied by AFM and NR the critical denaturation temperature (T_{cd}) for recrystallized S-layers on PE cushion. The change in the film density and thickness of the recrystallized S-layer was monitored as a function of the temperature and also the reversibility of the S-layers structure after a gradual increase and decrease of the temperature in the range below T_{cd} was investigated.

The surface topography of the two-dimensional S-layer structure recrystallized on polyelectrolyte multilayers was imaged in liquid, operating in contact mode (scan rate 4.70 Hz, at a force about 0.7-1 nN) with a multimode atomic force microscope Nanoscope III (Veeco Instruments Santa Barbara, CA). The NR experiments were performed with the solid/liquid experimental cell, at the time-of-flight neutron reflectometer AMOR at SINQ/PSI. Silicon blocks preliminary covered using the LBL technique [4] with a negatively charged PEM consisted of poly(sodium 4-styrenesulfate) (PSS) and poly(allylamine hydrochloride) (PAH) and an initial layer of poly(ethyleneimine) (PEI) were used. The sample was PSS-terminated. S-protein was in-situ adsorbed. The complex built has been exposed at different temperature steps: NR experiments started at room temperature against D₂O to different elevated temperatures (25, 35, 45, 50, 55, 60, 65 °C). The temperature was decreased in the same order down to room temperature to test the reversibility of the protein structure upon temperature treatment.

Probing protein denaturation

AFM deflection images showed that recrystallized S-layers on a polyelectrolyte multilayer (PSS terminated) are denaturated after 10 minutes exposure to 55°C (Figure 1). The 2-D crystal-line pattern (Figure 1, left) is lost (Figure 1, right). NR measurements (Figure 2) show a shift to the left of the fringe at 55°C (curve 3), which is explained by a decrease in the S-layer thickness of 1.8 nm. The increase in the SLD (5.39) at 55°C compared with the SLD (4.97) at 25°C, shows a decrease in

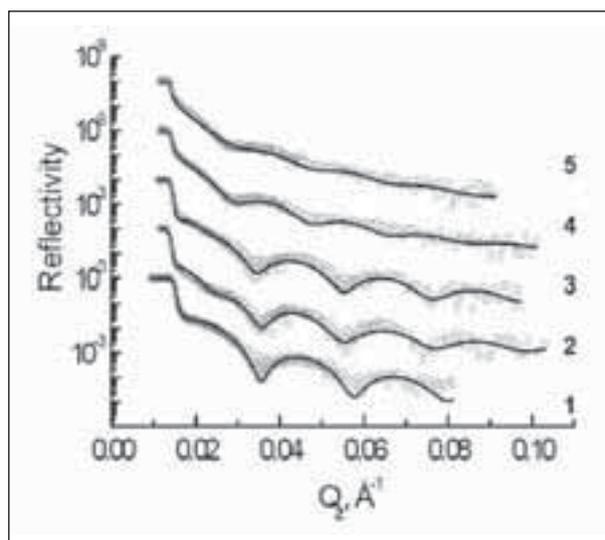


Figure 2: **Reflectivity curves at different temperatures.**

- 1) Si/PEI/(hPSS/PAH)6/hPSS bare support at 25°C,
- 2) Si/PEI/(PSS/PAH)6/PSS/S-layer at 25°C, 3) at 55°C, 4) at 60°C, 5) at 25°C.

the density of S-layer, which can be explained by structure denaturation. The temperature of 55°C is considered the critical denaturation temperature (T_{cd}) and the structure of recrystallized S-layer cannot be recovered by decreasing the temperature (curve 5).

Both AFM and NR results show that S-layer structure is lost at 55°C (the critical denaturation temperature). Further decrease in the temperature or treatment with recrystallization (Tris-HCl buffer, pH 9, with CaCl₂) cannot recover the 2-D S-layer structure.

The present work opens two approaches i) physico-chemical approach in order to get a hint about what holds the protein layer on the surface and to elucidate the influence of the temperature on the number of crystal defects, and ii) technological approach for the adsorption/immobilization of nanoparticles on the S-layer pores followed by the S-layer denaturation in order to study the trap of such nanoparticles.

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Radiolabelled, neurotensin analogues in human colon cancer-bearing mice

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Neurotensin (NT) receptors are overexpressed in several human cancers and can be used as targets for tumour diagnosis and therapy with radiolabelled NT analogues. The stable analogues NT-XII and NT-XIX allowed tumour localisation by SPECT/CT after labelling with the radionuclides Tc-99m and Re-188. Moreover, both analogues labelled with Re-188 inhibited the tumour growth in a model of human colon cancer-bearing mice.

Neuropeptide receptors are expressed at high concentrations in a variety of human malignant tissues and represent interesting targets for tumour imaging and therapy. It has been reported that neurotensin (NT) and its high affinity receptor (NT-1 receptor) are involved in several neoplastic processes, such as proliferation of pancreas, prostate, colon and lung cancer cells [1], protection against apoptosis in breast cancer cells [2], or progression of breast cancer [3]. The rapid degradation of the natural sequence of NT is a limiting factor that precludes its use in clinics. Therefore, stable, radiolabelled NT analogues may be good radiopharmaceuticals for targeting NT receptor-overexpressing tumours. New derivatives were synthesised with modifications in the amino acid sequence, which resulted in an important increase of the metabolic half-life without significant loss of the affinity to the receptors. The analogues NT-XII and NT-XIX that include changes at two and three cleavage bonds, respectively, seem excellent candidates for diagnosis and therapy (sequences in Figure 1).

Biodistribution and SPECT/CT studies

Stable ^{99m}Tc -labelled NT analogues were tested *in vivo* in mice with HT-29 tumour xenografts, a human colon adenocarcinoma cell line that overexpresses NT receptors. They showed higher specific tumour uptake and much better tumour-to-background ratios than non-stabilised analogues [4-6]. The xenografts were also clearly visualised by scintigraphy in the mouse model.

Moreover, one of the stable NT analogues was tested in clinics and allowed the detection of the tumour in a patient with a pancreatic adenocarcinoma that expressed high amounts of NT receptors [7]. The analogues NT-XII and NT-XIX showed the best biodistribution after labelling with Tc-99m. A compa-

table biodistribution was obtained with these derivatives labelled with Re-188 (Figure 1).

Scintigraphic images were acquired in mice with HT-29 tumour xenografts with a small animal SPECT/CT camera. The tumours could be clearly localised with both NT-XII and NT-XIX, either in the ^{99m}Tc - or the ^{188}Re -labelled form (Figure 2). Kidney and liver uptake was lower for the analogue NT-XIX, as compared with NT-XII, confirming the results found in the biodistribution studies.

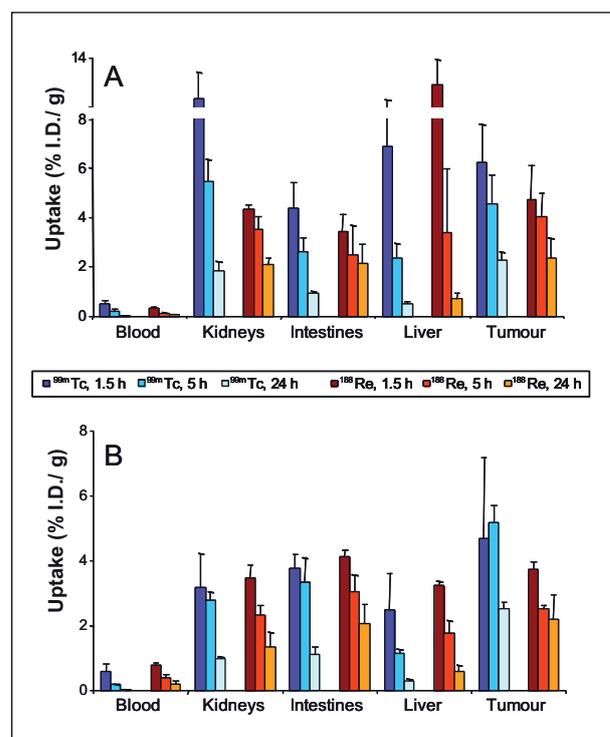


Figure 1: Comparison of the biodistribution of ^{99m}Tc -labelled and ^{188}Re -labelled NT analogues.

A) NT-XII [(N^εHis)Ac-Arg-NMeArg-Pro-Tyr-Tle-Leu].

B) NT-XIX [(N^εHis)Ac-Arg-NMeArg-Pro-Dmt-Tle-Leu].

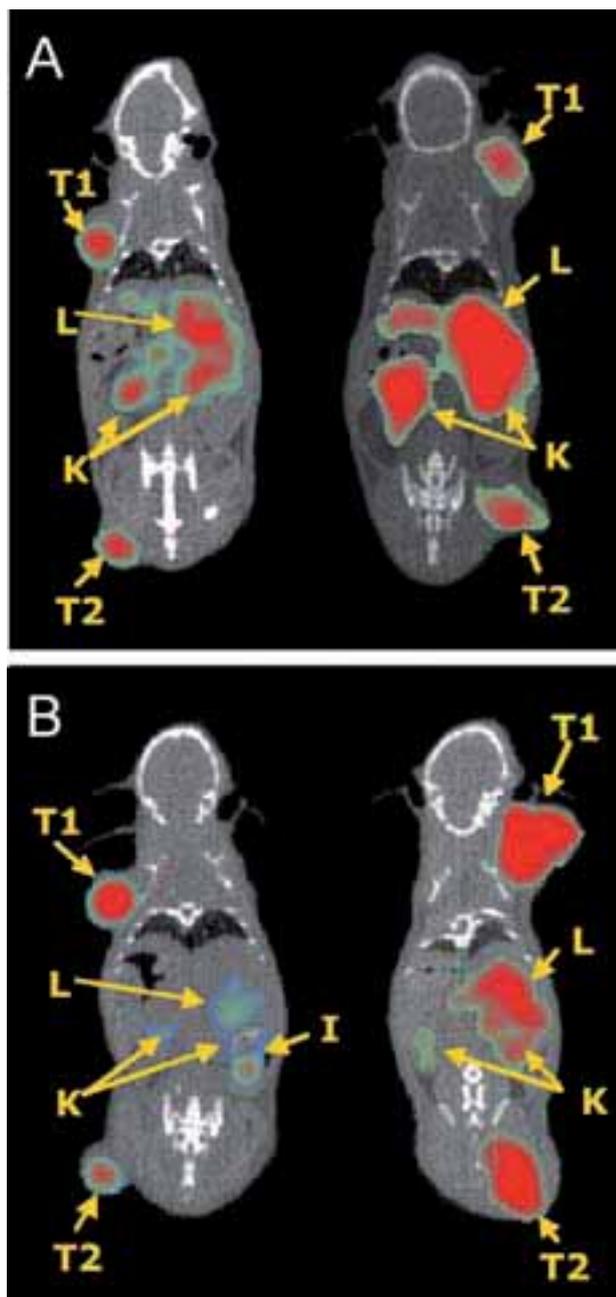


Figure 2: Coronal sections of the SPECT/CT images of ^{99m}Tc - and ^{188}Re -labelled NT analogues.
 A) NT-XII. T1 and T2 = tumours; L = liver; K = kidneys; I = intestine.
 B) NT-XIX. T1 and T2 = tumours; L = liver; K = kidneys; I = intestine.

Therapy studies

NT-XII and NT-XIX showing the best *in vivo* properties were selected for a therapy study after labelling with Re-188. The test was carried out in mice with HT-29 xenografts. Both ^{188}Re -NT-XII and ^{188}Re -NT-XIX, injected in two fractions of 15 MBq/mouse (total accumulated dose = 30 MBq/mouse) inhibited the growth of the tumour xenografts (Figure 3). In addition, ^{188}Re -NT-XIX, administered three times at a dose of 10 MBq/

mouse (total accumulated dose = 30 MBq/mouse) also showed a similar inhibitory effect in tumour growth. The lower kidney and liver uptake of this analogue would entail lower risk of radiation toxicity in these organs, which will therefore increase the potential of NT-XIX as radiotherapeutic.

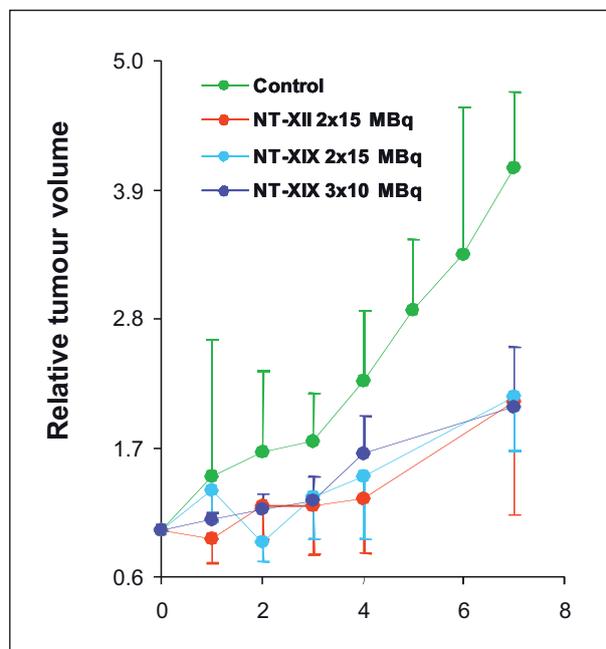


Figure 3: Effect on tumour growth in mice bearing HT-29 xenografts. Mice were injected with the ^{188}Re -labelled analogues at day 0 and 2 (2x15 MBq/mouse) and at days 0, 2 and 4 (3x10 MBq/mouse).

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^{67}Cu -Radioimmunotherapy in a mouse model of human ovarian cancer metastases

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The growth-promoting and anti-apoptotic properties which the L1-CAM cell surface protein confers to tumour cells give a rationale for antibody-based therapies. We investigated effects of radioimmunotherapy with ^{67}Cu -labelled anti-L1 antibody on growth of human ovarian cancer metastases in nude mice. In this model system for aggressive metastatic ovarian cancer, tumour reductions with single intravenous injections of 4 MBq or 10.5 MBq of the ^{67}Cu -antibody were found to be similar (about 70-80%) and ascites formation was inhibited by both radiocopper conjugates. Survival was only increased significantly with the 10.5 MBq dose. We found that when a single 4 MBq dose of ^{67}Cu -chCE7agl was combined with biweekly doses of growth inhibiting anti-L1 antibody L1-11A, which targets a different epitope on L1 than mAb chCE7, survival was prolonged significantly.

L1 expression in ovarian tumours

The list of tumours exhibiting overexpression of the L1 cell adhesion molecule (L1-CAM) keeps growing. In the recent immunohistochemical survey of Huszar et al. [1], a large number of benign and malignant tumours of the female genital tract were investigated for L1 expression. Both epithelial type tumours of the uterus and of the ovaries expressed L1. The results underlined prevalence of L1 in ovarian carcinomas: all (100%) of the tested serous (60/60) and clear cell (15/15) ovarian adenocarcinomas were L1 positive. The growth promoting and anti-apoptotic properties which L1 expression confers to tumour cells (reviewed in [2]) give a rationale for anti L1-based therapies. We showed recently that L1 is a valuable therapeutic target because anti-L1 antibodies suppressed tumour growth and ascites formation in a metastases model for human ovarian cancer [3]. In this study biweekly injections (10 mg/kg doses) of anti-L1 mAb L1-11A led to an about 50% reduction in tumour mass. When sections of orthotopically implanted SKOV3ip human ovarian cancer cell metastases were stained with anti-L1 mAb 14.10 we observed surprisingly heterogeneous expression of L1. Figure 1 shows immunohistochemical staining of tumour tissue from untreated animals, showing areas with L1 negative tumour cells and L1 positive cells (red-brown) in the leading edge of the tumour and in tumour cells invading the muscle tissue. The crossfire of radioimmunotherapy with beta particle emitting nuclides spans over many cell diameters and can hit tumour cells which do not express the L1 target.

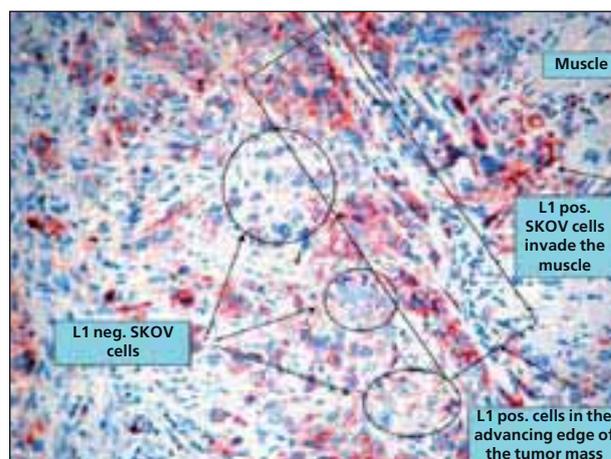


Figure 1: Immunohistochemical staining of a section from abdominal SKOV3ip tumour mass.

^{67}Cu -Radioimmunotherapy

We assessed anti-tumour effects of single doses of ^{67}Cu -CPTA-labelled anti-L1 antibody chCE7. An aglycosylated variant form of chCE7 antibody (chCE7agl) was produced in HEK293 cells, which combines a more rapid clearance from the blood with a similar high uptake in tumour than the parent mAb chCE7 [4]. chCE7agl was labelled with PSI-produced ^{67}Cu using the CPTA chelate to a specific activity of about 16 MBq/mg. Two days post-intraperitoneal implantation of SKOV3ip cells two different doses of ^{67}Cu -CPTA-chCE7agl were applied as single intravenous injections in groups of 8-9 animals. After 23 days

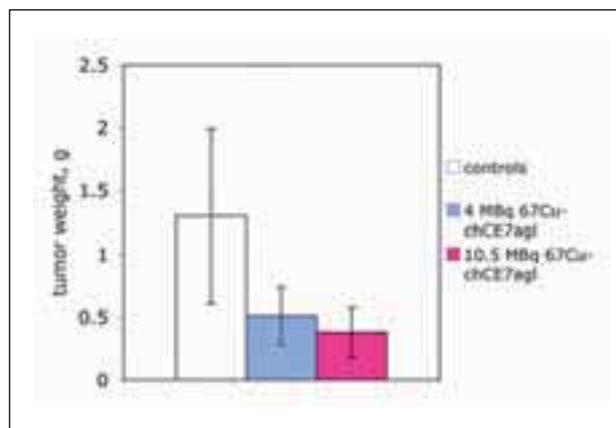


Figure 2: L1-directed therapy of orthotopic SKOV3ip tumours in nude mice treated with a single dose of ^{67}Cu -chCE7agl.

the animals were euthanised and the abdominal tumour masses were removed and weighed. The extent of ascites in the abdominal cavity, which is a hallmark of late stage ovarian cancer, was also measured. We found that 7 of the 11 untreated animals presented with ascites, whereas no ascites was found in the animals treated with low dose ^{67}Cu -RIT and 2 of the 9 animals in the group receiving high dose ^{67}Cu -RIT showed ascites. Figure 2 shows that both single low dose and high dose ^{67}Cu -RIT reduced the tumour size significantly ($P=0.003$ and 0.006 respectively) about 60-70%.

The decrease in tumour mass observed by single-dose radioimmunotherapy or by repeated administration of unlabelled anti-L1 antibodies may not necessarily lead to increased survival. We therefore designed experiments to investigate survival using ^{67}Cu -labelled chCE7agl alone and in combination with unlabelled anti-L1 mAb L1-11A. L1-11A targets a different

epitope on the L1 protein and does not interfere with binding of mAb chCE7. We found that the low 4 MBq dose of ^{67}Cu -labelled chCE7agl did not prolong survival significantly, in contrast to the 10.5 MBq dose, which led to a significantly increased survival.

Figure 3 top shows Kaplan-Meier plots of the survival of groups of animals ($n=7-8$) inoculated with SKOV3ip cells which received two days later a single i.v. dose of either 8 MBq ^{67}Cu -CPTA-Lym1 antibody (nonbinding control) or 10.5 MBq ^{67}Cu -CPTA-chCE7agl antibody. Treatment with ^{67}Cu -CPTA-chCE7agl showed significantly longer survival than no treatment (controls) ($P=0.0335$), whereas the nonbinding control antibody had no significant effect. The lower graph in Figure 3 shows the survival curves for animals treated with low dose ^{67}Cu -Lym1 control antibody or ^{67}Cu -chCE7agl, which were found to be not significantly different from the untreated control. In contrast the combination of a single low dose of ^{67}Cu -RIT with biweekly doses of anti-L1 mAb L1-11A increased survival significantly over controls ($P=0.0063$) and over the group with single low dose RIT by itself ($P=0.046$).

Results

These results show the feasibility of setting up combination therapies with radiolabelled and unlabelled anti-L1 antibodies, with the aim to enhance the efficacy observed with the single treatments.

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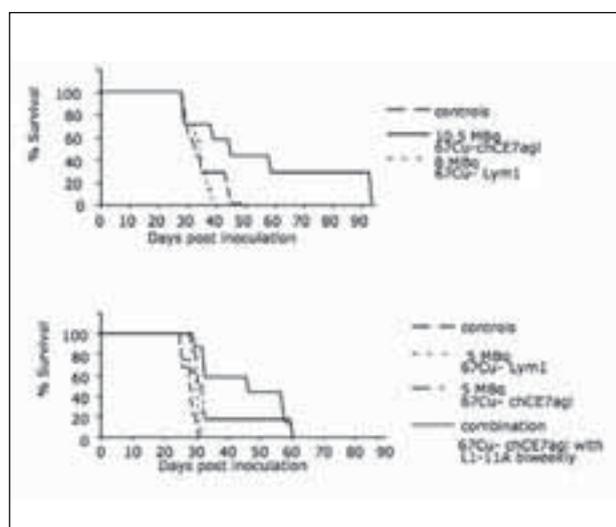


Figure 3: Kaplan-Meier survival plots after ^{67}Cu -radioimmunotherapy, as single treatment or in combination with biweekly administration of unlabelled anti-L1 antibody.

Progress on advanced scanning in the Gantry 2 test area

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In a first phase a test area was operated during the commissioning of the COMET accelerator to measure important proton beam parameters. In a second phase the test area was used to explore new scanning techniques and to develop part of the new control system for Gantry 2. During this stage two sweeper magnets for fast proton beam scanning were installed in the beamline. We implemented the spot scanning mode and we showed the feasibility of some advanced scanning techniques like simulated scattering and intensity modulation including fast energy variations with the beam.

Introduction

During commissioning of the COMET accelerator and PROSCAN beamline a test area was installed close to the coupling point of the future Gantry 2. One purpose of this test area was to measure the proton beam characteristics of COMET at the end of the beamline.

At the same time as Gantry 1 was connected to the new accelerator, two sweeper magnets were inserted in the beamline of the test area – a simplified setup of the new Gantry 2. The two magnets allow a fast proton beam scanning with up to 2 cm/ms at the planned patient position in two dimensions and they have been the ideal platform to develop the control system and to test scanning strategies.

Experimental setup

For patient treatment the typical proton energy ranges from 70 MeV to 250 MeV. In a first step an appropriate set of these energy tunes had to be found. Since the degrader's transmission of low energies decreases by two orders of magnitude compared to high energies, we had to find a way to keep the final beam intensity constant for all energies. This requirement was achieved by introducing an energy-dependent beam defocusing with quadrupoles on a collimator. As an additional benefit, changing the beam tune in typical steps of 3 MeV was still fast, since no mechanical devices had to be moved, and could be performed within 90 ms.

The intensity of the beam was measured by a fast ionisation chamber (IC). The lateral displacement of the 10 mm wide spot was observed with a CCD box. In this box a CCD camera was focussed on a scintillation foil which was mounted perpendicular to the initial proton beam (Figure 1). To observe the dose distribution in different depths a stack of Plexiglas plates could be inserted.

Results and conclusion

First we implemented the spot scanning mode in which a dose distribution is built up by applying discrete dose spots similar to Gantry 1. The dose per spot was calculated [1] in such a way that the homogeneous dose distribution of 1.2 Gray formed a cube of 8 cm in a water equivalent depth of 10 to 18 cm. The cube consisted of 5491 spots, which were applied in 40 s. Since the dose of each spot was controlled by the IC the reproducibility and homogeneity was better than 1% (Figure 2).

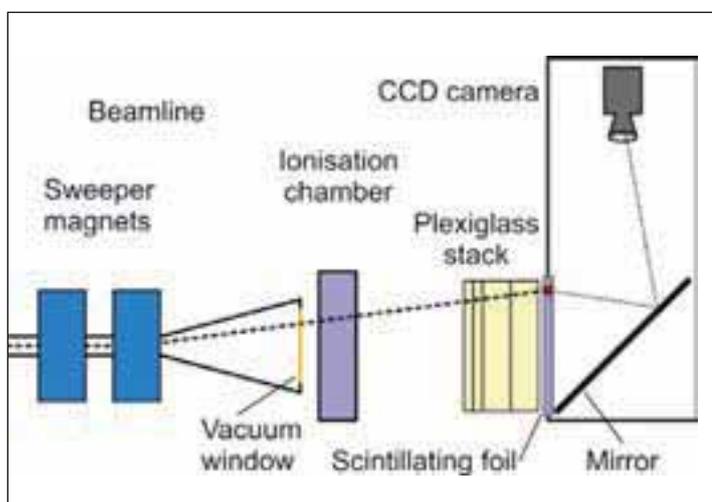


Figure 1: Experimental setup in the test area.

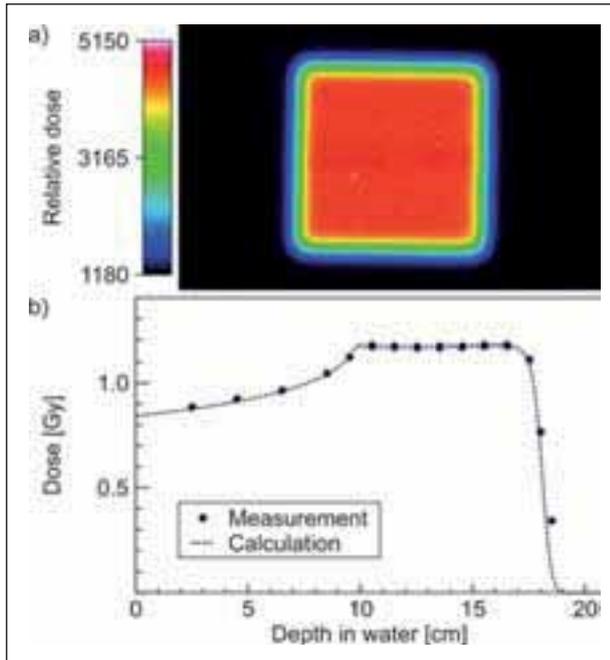


Figure 2: CCD image of a cubic dose distribution applied with spot scanning at 1 cm water equivalent range (a) and the measured depth profile compared to calculation (b).

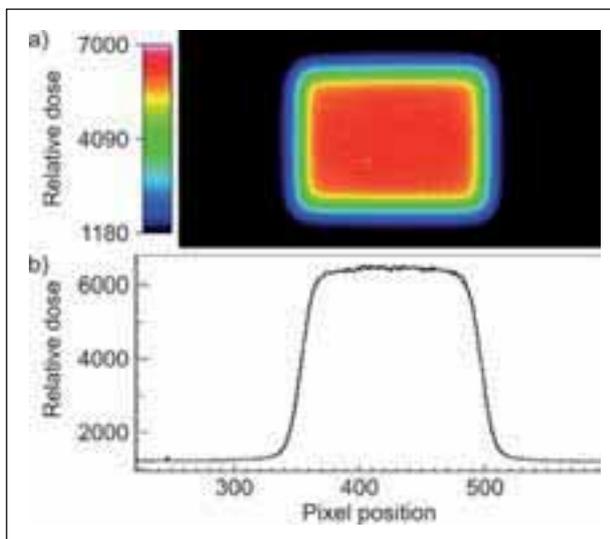


Figure 3: CCD image of a cubic dose distribution at 12 cm water equivalent range using simulated scattering (a) and its horizontal profile (b).

The same technique was used in the Absolute Dosimetry Project with a water calorimeter, which is also described in this report (p. 60).

In a next step the dose was deposited in a so-called simulated scattering mode. In this mode one energy plane is applied by painting a meander pattern with continuous proton beam at the sweeper magnets maximum speed.

In order to deposit 1 Gray in a similar cube of $8 \times 6 \times 8 \text{ cm}^3$ the energy planes were repainted in total 494 times, which required about 50 s. Due to the large number of repaintings the fast intensity fluctuations of the proton beam were statistically compensated and the homogeneity of the dose was quite as good as for spot scanning, even though the intensity was not controlled (Figure 3). The control of the overall dose was not yet addressed for this mode.

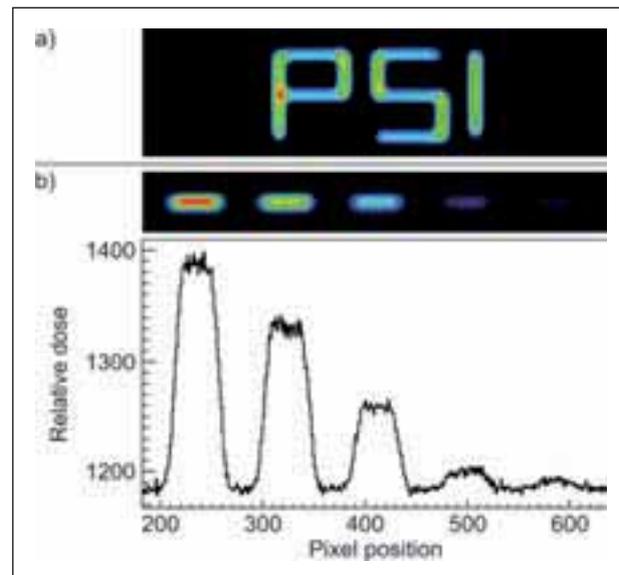


Figure 4: CCD image of PSI logo using continuous line scan, applied in 80 ms (a); and an intensity modulated line with its profile, applied in 30 ms (b).

Finally, some aspects of advanced scanning modes were tested. In these modes the proton beam will no longer be limited to horizontal or vertical lines and the intensity will be modulated at high speed with help of the vertical deflector plate inside the COMET cyclotron (Figure 4). One of the challenges in these modes is to synchronize precisely all actuators – a task which was successfully handled by the control system.

In all three modes the architecture of the control system showed its flexibility and the existing hardware allowed a precise, three-dimensional dose application. Due to the actual 15% dead time for a cubic dose distribution the dose was also applied efficiently.

The test area was closed at the end of year 2006 and developments will restart on Gantry 2.

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Absolute dosimetry of scanned protons with a water calorimeter

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When using ionizing radiation for therapy, the dosimeters have to be traceable to national primary standards. Primary standards for dosimetry exist for photons and electrons, however no direct internationally recognized primary standard exists yet for therapeutic proton beams. This report describes the first results obtained with a water calorimeter exposed to scanned protons in the PROSCAN test area in December 2006.

Dosimetry in proton therapy

In radiotherapy, the absorbed energy in a tissue is defined in terms of the absorbed dose to water D_w (SI units Gy = J/kg). The conventionally used ionizing chambers have to be traceable to a primary standard. A water calorimeter is the preferred primary standard as it directly measures the temperature rise induced by the energy deposited owing to the absorbed dose in water. This approach requires sensitive thermometry as the temperature rise is only 0.238 mK per Gray. In addition, the water has to be ultra pure in order to reduce the major uncertainty of this primary standard: the chemical heat defect

owing to irreversible radiochemical processes which will not show up in the temperature rise [1]. METAS has realized a water calorimeter to be the Swiss primary standard for therapy dosimeters in conventional high-energy photon therapy [2,3]. As no internationally recognized direct primary standard for D_w in proton therapy exists yet (today the dosimeters used in proton therapy are traceable to Co-60 beam quality with calculated correction factors for protons), PSI and METAS have decided to join efforts in order to realize such a primary standard [4]. Here we report on the first experimental results using a replicate of the standard METAS water calorimeter in the PROSCAN test area in December 2006.

Experimental setup

The water calorimeter consists of a sealed glass vessel (diameter 6 cm) containing two NTC thermistors (10 k Ω at 4 $^{\circ}$ C) inside a water phantom of 30 cm side length. The water phantom is inside a thermally insulated wooden box in which cooled air is circulated. The temperature of the water phantom is kept at 4 $^{\circ}$ C (maximal water density) in order to minimize convection. The water calorimeter has been placed in the PROSCAN test area and homogeneous 3D box dose profiles were deposited in the water phantom. Typically the box was 8 x 8 x 8 cm³, centred at a point located 15 cm downstream from the phantom entrance window, the approximate position of the thermistors in the glass vessel. Figure 1 shows the experimental setup schematically.

The resistance change of the thermistors owing to the temperature rise induced by the absorbed dose is measured with a Wheatstone bridge and a phase sensitive lock-in amplifier, leading to a temperature sensitivity of 10 μ K.

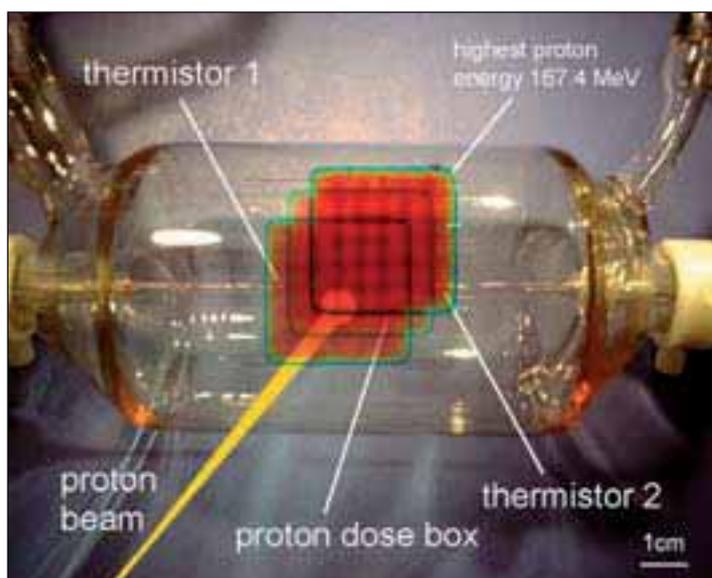


Figure 1: The sealed vessel of the water calorimeter with two thermistors separated by 1 cm. Superimposed is a schematic scanned proton dose profile.

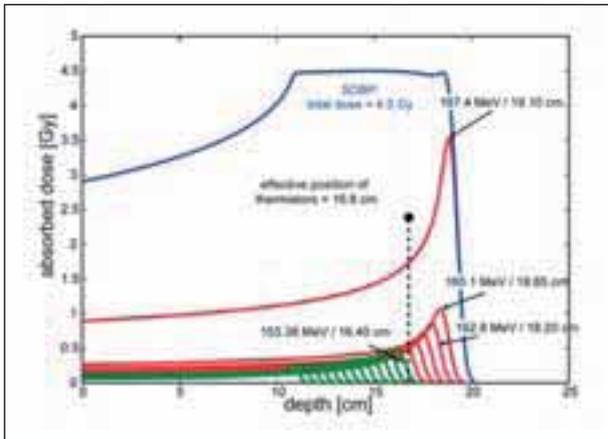


Figure 2: **The SOBP of a 4.5 Gy dose box in the water phantom (8cm x 8cm x 8cm box centred at 15 cm).**

Experimental results

Using the spot scanning technique [5], pencil beams with a gaussian width of $\sigma = 4.5$ mm were deposited in a plane perpendicular to the beam direction at given water depth determined by the energy of the pencil beam. The distance between the x-y spots in a given water depth was 5 mm. In order to create a homogeneous box with a flat SOBP, the dose of the proton pencil beam corresponding to a given energy plane (water depth) was determined by a calculated weight factor. The distance between the energy planes in the water phantom corresponds to 4.5 mm. Figure 2 shows the individual dose profiles for the 19 energies required to create an 8 cm box with a flat SOBP corresponding to 4.5 Gy. The thermistors recorded a temperature rise for dose deposition of the first six energy planes. No signal was seen for protons with an energy of 153.38 MeV, corresponding to a Bragg peak maximum at 16.4 cm. This indicates that the geometrical 3D dose profile has a rather sharp cut-off in water at 4 °C owing to the small heat conductivity of water of $0.61 \text{ Wm}^{-1}\text{K}^{-1}$. The proton beam current was such that the deposition of a 4.5 Gy in an 8 cm box took 80 seconds. In Figure 3 the temperature rise of the two thermistors is shown for the 4.5 Gy 8 cm box. Although the first energy plane has its Bragg peak at a depth some centimetres larger than the position of the thermistors, a dose is deposited in the proximity to the thermistors owing to the plateau of the dose profile as shown in Figure 2. Because the two thermistors are separated by 10 mm, a time difference of the onset of the temperature rise of 2.6 seconds is to be expected for the deposition of the deepest dose plane produced by the protons with energy of 167.4 MeV. The highest energy has the largest weight factor, leading to the strongest temperature rise. The arrival time of the pencil beams corre-

sponding to the smaller proton energies can be calculated from the various weight factors and magnet and energy switching times. As can be seen in Figure 3, these times correspond reasonably well with the observed onset of the various temperature rises. A deposition of 4.5 Gy in water at 4 °C leads to a temperature rise of 1.07 mK, a value which is also reasonably well measured by both thermistors. In order to use the water calorimeter as a primary standard for scanned proton beams, the various parameters will now have to be studied systematically, notably the heat defect, which is typically the largest uncertainty in the water calorimeter. The results presented in this report demonstrate that the 3D dose profile produced by the spot scanning technique of PROSCAN is sufficiently long-lived in water that absolute dosimetry with a water calorimeter should be feasible.

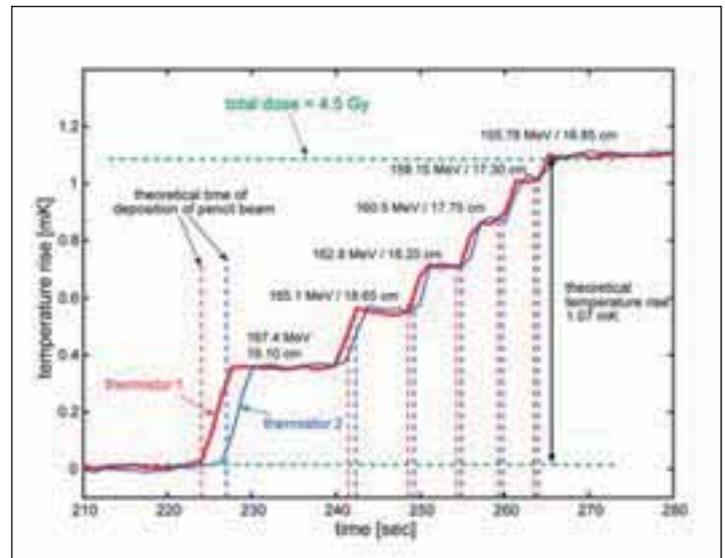


Figure 3: **The temperature rise signal of the two thermistors for the cubic dose distribution of 4.5 Gy.**

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Commissioning and preparations for patient treatment with COMET (PROSCAN)

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The superconducting 250 MeV cyclotron COMET for PSI's new proton therapy facility PROSCAN has been commissioned and handed over to PSI after having successfully passed the majority of the acceptance tests. The beamline to the test area was used until December 2006. After installation and commissioning of the beamline to Gantry-1 the preparations and tests for patient treatments were started.

Introduction

Parallel to the acceptance tests of the cyclotron, an extensive measurement programme has been carried out to study the characteristics of the cyclotron and the beamlines. In August 2006 the final preparations for patient treatment with Gantry-1 were started. The full simulations of treatments started in December 2006.

Acceptance tests of the cyclotron COMET

After the delivery and commissioning, the SC cyclotron COMET was subject to a rigorous test program. In 2004 PSI had defined 37 acceptance tests. In December 2006, 33 of the tests had been performed successfully, and PSI could formally take over the cyclotron. These tests and the final commissioning of the cyclotron were performed in close collaboration with the manufacturer ACCEL Instruments GmbH (D). In addition to tests on beam characteristics [1], the reliability of the cyclotron

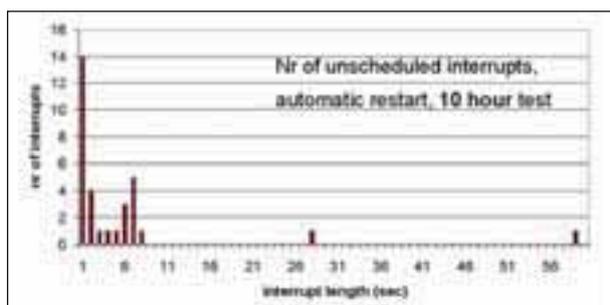


Figure 1: **Unscheduled interruptions during a test of 10 hours' running time.**

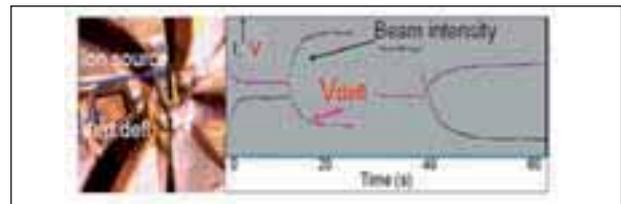


Figure 2: **The vertical deflector used for intensity control and beam on/off switching.**

was tested. Figure 1 shows the number of unscheduled beam interruptions of different lengths, during a 10-hour run. The number of long interruptions (2) and the total time without beam (3 min.) were well within the specifications.

A vertical deflector in the centre of the cyclotron can be used for beam-intensity control (Figure 2) or as a fast on/off switch (40 μ s). The stability of the beam intensity is just sufficient for operation with Gantry-1 but it fluctuates too much in the millisecond time scale for Gantry-2 operation. Therefore a development programme to improve the beam stability has been started together with ACCEL.

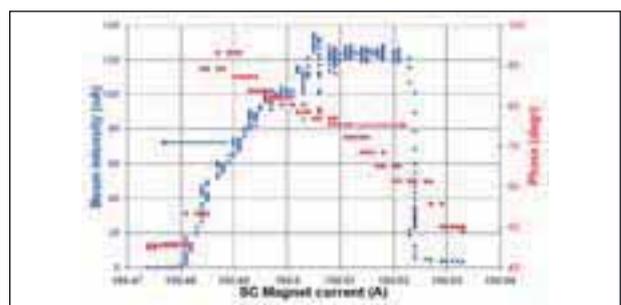


Figure 3: **Extracted beam intensity and beam phase as a function of the current in the SC coil.**

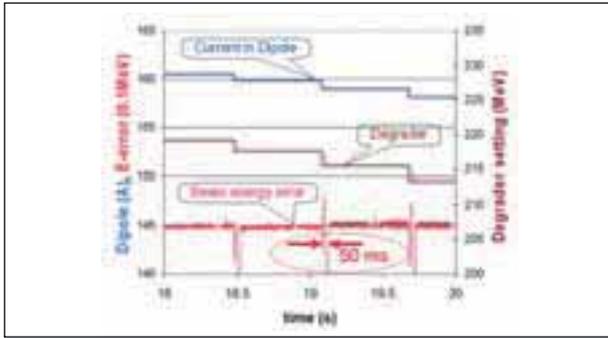


Figure 4: **Beam energy deviation in sequential beam tunes (220, 218, 216, 214 MeV), set within 50 ms.**

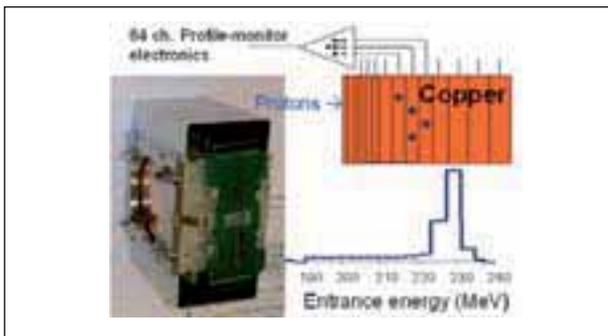


Figure 5: **Beam energy spectrum from the MLFC [2].**

In order to compensate the change of the magnetic field due to RF-heating of the iron, the magnetic field is corrected by stabilizing the phase of the extracted beam at $\sim 68^\circ$ (Figure 3). A stabilization loop is still needed, since the magnet current correction applied over a day can amount to 20–30 mA.

An important property of the cyclotron is the high extraction efficiency ($> 80\%$ routinely). After one year of operation, this has paid off in a low activation of COMET amounting to only a few mSv/h immediately after 500 nA and ~ 0.5 mSv/h, after 24 hours without beam. This considerably simplifies maintenance work at the cyclotron.

Commissioning of the beamline

The emittance of the extracted beam is matched to optimize the transmission, and maximize the beam suppression when the preceding kicker magnet is used to switch the beam off. The energy of the extracted beam is reduced to the desired energy by means of the fast degrader system developed at PSI.

The most important feature (for fast scanning with the new Gantry-2) of the beamline system of PROSCAN is the capability to adapt within 50 ms to the beam energy changes from the degrader between 67 and 235 MeV in steps of 2%. Using a set of different beam energies (*tunes*), we have tested this capability by measuring the degrader setting, the magnet current of the first 45° dipole and the beam energy error, while switching rapidly between tunes (Figure 4). For detailed stud-

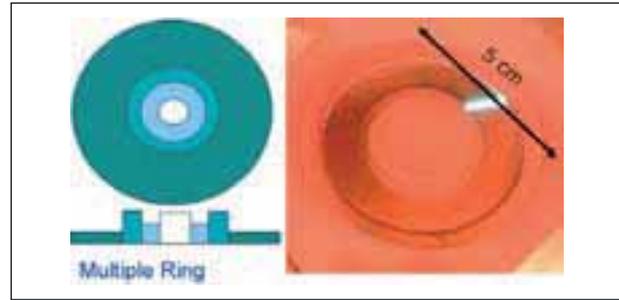


Figure 6: **A foil consisting of multiple rings is used as second scatter foil for OPTIS-2. The foil is made by laser ablation at the University of Applied Sciences, Aargau (CH).**

ies of the beam energy dependence from various machine parameters, we used a Multi Leaf Faraday Cup (Figure 5).

On June 9, after the shutdown to connect Gantry-1 to COMET, the beam was sent to the gantry isocenter and we could commission the dedicated on-line tune verification diagnostics at the Gantry-1 coupling point. A good agreement was observed between the measured beam sizes and the beam optics calculations.

For the new eye treatment facility, OPTIS-2, a novel dual scattering technique has been designed to optimize the beam transmission to the tumour volume. Using a multiring foil in a dual scattering system, the proton beam entering the vault will be used 20–50 times more efficiently than in the current OPTIS setup. Therefore, despite the much lower beam intensity, we can keep almost the same treatment times as before.

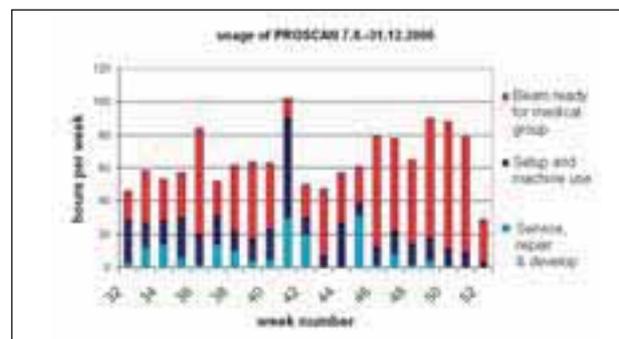


Figure 7: **Beam time use since August 2006.**

Outlook

The first months of operation have shown that the facility is sufficiently reliable and stable for patient treatment. The time used for machine development and repairs has decreased steadily and since December 2006 the facility is almost 100% used by the Radiation Medicine department to prepare and test the patient treatment procedures. These preparations will finish in February 2007. In June 2007 Gantry-2 and OPTIS-2 will be installed.

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Installation of the new proton therapy unit – Gantry 2

Eros Pedroni *for the Gantry 2 team of PSI*

The installation of Gantry 2 was started in 2006. Gantry 2 is based on a double-parallel magnetic scanning and has been designed for dedicated use of the intensity modulation at the ion source of the new accelerator COMET and for fast dynamic changes of the beam energy with the PROSCAN degrader ahead of the gantry. The goal is to develop new advanced beam scanning techniques for treating moving targets with dose repainting. The long-range development program includes simulated scattering – gating – tracking – and image-guided proton therapy using beam eye view X-rays taken simultaneously to the proton beam.

Project goals

While Gantry 1 will fulfil the main role of treating patients at PSI as it has done in the past, Gantry 2 is being built within the project PROSCAN as the new instrument for performing further developments of the beam scanning technology, the proprietary speciality of PSI in this field. We aim to achieve faster beam delivering techniques in order to be able to apply pencil beam scanning with repainting so that we can treat tumors in the whole body including moving targets, such as tumours in the chest.

Status of Gantry 2

The rotating support of Gantry 2 was delivered by the company Schär Engineering AG in August 2006.

The most crucial component of the gantry beamline is the 90° bending magnet, which arrived at PSI on the 26th of December. Figure 1 shows a photograph of this 35-ton heavy ‘Christmas gift’.

Figure 2 shows the support after installation in the area. The new system rotates from -30° to 180° in the vertical only on one side and is supported on a central U-shaped pivot. The gantry layout is optimized for a functional and patient-friendly setup on a permanent fixed floor.

The achievements of 2006 in developing advanced scanning techniques in the provisional test area of PROSCAN are described in other articles in this report.

The test area was dismantled in January 2007 in order to connect the Gantry 2 area with COMET (completion planned for June 2007). The mounting of the beamline section of the gantry will follow in summer 2007.



Figure 1: 90° bending magnet (delivered by Sigmaphi).

In spring we should receive the patient table and mount the components of the nozzle. First protons through the Gantry 2 are expected before the end of 2007.

Figure 2: Gantry pieces are set into position.

(Photo: Beat Gerber)



Innovative magnet design for PROSCAN

David George, *Department of Large Research Facilities*; René Künzi, *Power Electronics, PSI*

The PROSCAN project at PSI involves a number of innovative elements. Apart from the compact superconducting dedicated cyclotron COMET, a fast degrader and laminated magnets in the beamlines, including the newly conceived Gantry-2, will enable rapid energy changes to modulate the range of the scanning pencil beam in the patient. The last multifunctional bending magnet of the Gantry-2 transport system and its power supply are not only the largest, but also the most challenging elements.

Magnet design

Since the magnet will be suspended in the gantry, the weight and bending radius should be minimized. The steady state magnetic design was performed using the POISSON code together with our own OPTIMA routines.

The most difficult requirement is for fast switching. Even though the magnet is manufactured using insulated iron laminations, the switching delay problem caused by eddy currents has to be studied in detail. The main problems occur in the entrance and exit regions, where the magnetic field does not necessarily follow the lamination pattern. We applied the Vector Fields ELEKTRA code to study the 3-dimensional eddy

currents in the anisotropic iron. The first calculations confirmed our fears. We could also verify the results with tests performed on the conventional PROSCAN dipoles [1]. It became clear that the eddy current problem is very serious at higher magnetic fields. However, if the fields are reduced, the magnet (and the gantry) becomes larger and heavier. A compromise had to be made at an early stage of the design so as not to compromise the Gantry-2 schedule. A first attempt to reduce the eddy currents using strategically placed slits in the iron proved to be insufficient. We finally adopted a radical approach by machining away the steel in the problem region and replacing it with longitudinal laminations. Unfortunately, despite all the available modern technology, it was not possible to completely calculate such a complicated configuration. A secondary special aspect of this magnet is the vacuum chamber. Because of the beam scanning, the vacuum chamber has to be much larger than for the rest of the beamline. In order to avoid any problems with metallic walls and even reduce the air gap, we propose to use an integrated chamber made using glass-fibre reinforced plastic. The poles have to be vacuum-tight and serve as the upper and lower chamber walls. Sealing to the poles is done with conventional rubber O-rings and the pole sides are used to support the lateral vacuum forces.

Yoke manufacture

The magnet was manufactured by the specialist magnet company Sigma Phi in Vannes, France in close cooperation with PSI and Schär Engineering Ltd. in Flaach. Due to the given geometry and the large size, a rather complicated manufacturing process was followed. A very important aspect was the welding process, starting at the 1 mm lamination thickness and ending up at the 180 mm thick steel of the support blocks.

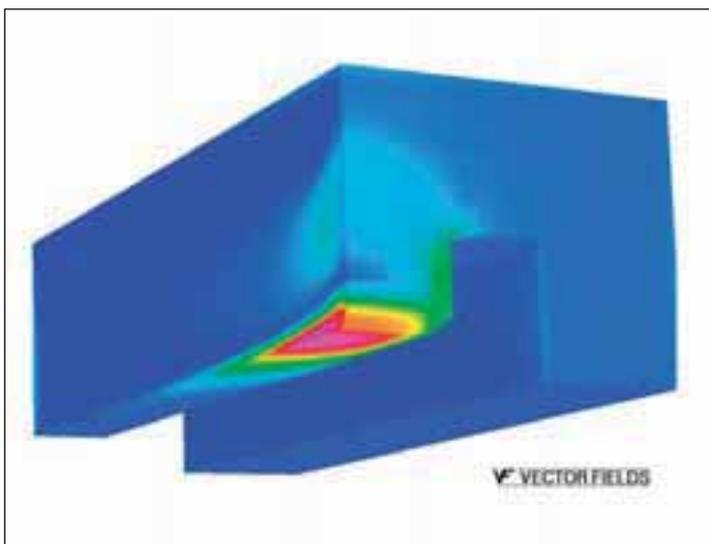


Figure 1: A simplified model of a laminated dipole showing the eddy current concentration at the pole end just before the currents travel like a wave towards the magnet centre. For simplicity, a 3-way symmetric model is used where only one-eighth of the magnet has to be modelled.



Figure 2: **One 23.5-ton half of the 90 degree magnet being prepared for shipping. The 1.9 ton coils are of conventional design and could be manufactured and test assembled into the iron yoke without any major problems arising.**

At the same time, the deformation of the steel body has to be controlled as far as possible. Following the final assembly, the pole surfaces were sealed by vacuum impregnation with epoxy resin.

Power supply

The power supply (PS) is designed for a max. output current of 500 A and output voltages of 180 V steady state and 350 V peak. The high dynamic requirements call for a 4-quadrant voltage source converter with pulse width modulation, the same concept as applied for all PROSCAN power supplies, but larger by a factor of three. The DC-Link, the converter and the output filters have to be designed for the peak output power of 175 kW, whereas the transformer must only be dimensioned for the steady state output power of 90 kW.

It is clear that a power supply with high dynamic requirements needs a high bandwidth in order to follow the current reference fast enough. From that point of view, the switching frequency should be as high as possible, but this increases the switching losses. The junction temperature should be kept low in order to maximize lifetime and availability. The converter operates at a switching frequency of 12.5 kHz and at semiconductor junction temperatures below 100°C, which is a rather conservative compromise. The controller is another speed-limiting component. For the entire PROSCAN beamline, we have used the same controller hardware as developed for the Swiss



Figure 3: **The heart of the 90°-dipole PS with the filters (upper level) and the 4-quadrant converter (lower level) packed into a radio frequency proof housing.**

Light Source (SLS) [2]. These controllers are powerful enough to fulfil the speed requirements. The 5 years of operational experience with approx. 580 PS in the SLS [3] show a very high reliability.

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General Energy Research Department: strategy and selected highlights

Alexander Wokaun, Samuel Stucki, Aldo Steinfeld, Peter Jansohn, Günther G. Scherer,
Research Department General Energy, PSI

General Energy research at PSI is contributing to Swiss and global goals for the development of a more sustainable energy system, focusing on two strategies. Firstly, the production of fuels from renewable primary energy aims to substitute scarce oil and gas resources, reduce the dependence on imported fossil fuels, enhance security of supply, and mitigate CO₂ emissions. Secondly, energy services should be rendered with the highest possible efficiency at minimum emissions.

The research portfolio

Four laboratories of General Energy focus on energy carriers from renewables and on efficient energy conversion; selected highlights are described in the sections below. The fifth laboratory, Atmospheric Chemistry, studies the fate of man-made pollutants in the Atmosphere (see Section 'Environment'). Energy Systems Analysis, a Laboratory operated jointly with the Nuclear Energy, Safety Department, evaluates life cycle inventories and risks of energy systems, and elaborates scenarios for the future development of the global energy system.

General Energy engages in the construction and operation of three beamlines at the Swiss Light Source. An important achievement was the recording of first light at the Infrared beamline in November of 2006.

Competence Center Energy and Mobility

The Competence Center for Energy and Mobility (CEM-CH) of the ETH Domain for which PSI acts as the facilitator, was launched in January 2006 (cf. page 70). After thorough evaluation of the proposals submitted fourteen projects have been approved that involve, besides partners from ETH Zurich, EPFL, and EMPA, several Universities of Applied Sciences, with strong participation by Swiss industry.

Researchers from General Energy are strongly involved in eleven projects of the Center. Mirroring the research portfolio, our contributions focus on the use of biomass for the production of second generation biogas, the production and the role of hydrogen in a future energy system, on advanced gas turbine processes, on the emission reduction of next generation large diesel engines, and on the niche market introduction of fuel cell vehicles.

Laboratory for Energy and Materials Cycles

New technologies target the production of fuels from biomass that meet the specifications of modern energy conversion processes. Research on fluidized bed catalytic reactors and gas clean-up processes has substantially contributed to finalizing the design of the first full-scale demonstration plant to convert wood to pipeline-grade synthetic natural gas (SNG). The plant will be built by our industrial partners in the first half of 2007.

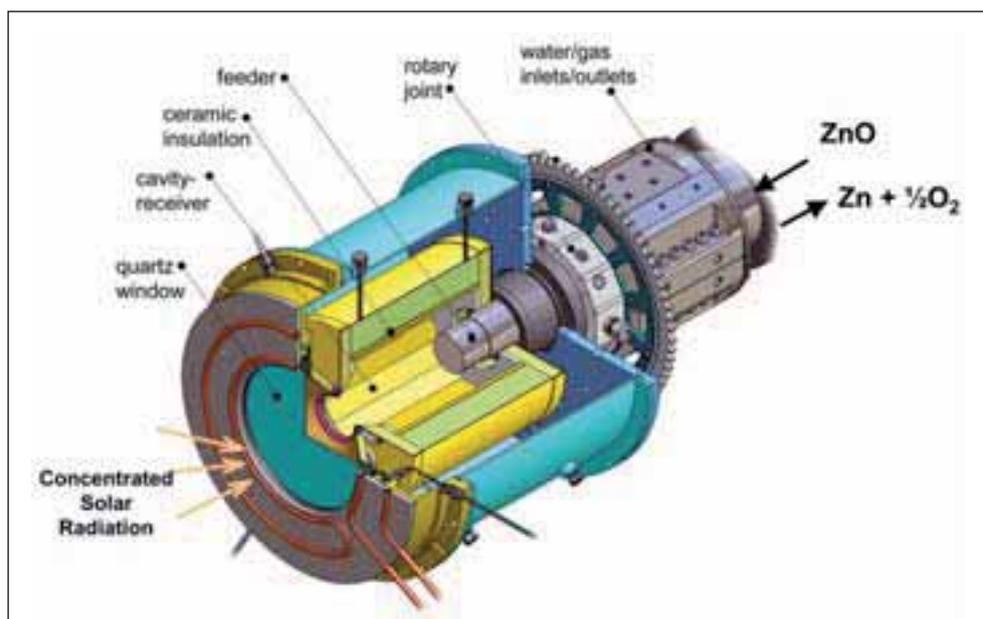
For the conversion of wet biomass, a 3 kW_{th} hydrothermal gasification/methanation test plant has been built to test the direct catalytic conversion of biomass to SNG. Progress has been made in salt separation and in understanding causes of catalyst deactivation.

For the direct conversion of gasified biomass to electricity, solid oxide fuel cells are a promising option. Our new pressurized counter-current gasifier will allow us to perform realistic long-term testing of fuel cell stacks in the 1 kW size. Of central importance for the success of biomass conversion to electricity or secondary fuels is the control of trace impurities. New techniques for quantitative analysis of trace components in real gases have been developed and are available for field testing.

Laboratory for Solar Technology

Energy-efficient production of solar fuels encompasses researching the fundamentals of thermochemical reactions and high-temperature solar reactor engineering. The accomplishments of 2006 advance our long-term goal of efficiently closing the 2-step water-splitting thermochemical cycle. Progress was

Figure 1: ZIRRUS; this solar reactor features a rotating cavity for the solar thermal dissociation of zinc oxide at temperatures above 2000 K.



made towards the solar reactor design for the thermal dissociation of ZnO at above 2000 K. We report on methodologies for investigating the rapid quench of the gaseous products for high zinc yield. The transition path to solar hydrogen is being pursued by the solar decarbonization of fossil fuels via cracking, reforming, and gasification processes.

Practical experience was acquired through the operation of our new high-flux solar simulator, which offers the world's highest performance level of combined radiative power (> 50 kW) and power flux (> 10,000 suns). It complements PSI's solar furnace in serving as state-of-the-art experimental platform for investigating solar thermochemical processes and testing advanced high-temperature ceramic materials. The synergy with ETH's Professorship of Renewable Energy Carriers enables us to optimize resources for accomplishing the challenging R&D goals of the efficient production of solar fuels.

Combustion Research Laboratory

Activities are centred on combustion systems which offer the highest efficiencies and lowest emissions, i.e. gas turbine-based processes and internal combustion engines. Besides application oriented research projects, the basics of physicochemical mechanisms for 'near zero emission' fuel conversion systems are studied.

In 2006 the molecular dynamics of important intermediate combustion species (partially oxidized hydrocarbons such as formaldehyde) were investigated in detail. A new fast laser diagnostics system enables us to study unsteady combustion phenomena at higher frequencies (kHz range) – the system will be applied to identify stability criteria for lean premix methane flames. With the addition of hydrogen and propane,

we have shown the flame stability and emissions characteristics of fuel mixtures that are potentially important in gas turbine processes of the future. Numerical studies on combustion fundamentals of catalytically supported combustors have been expanded to sub-mm scale reactors. The detailed knowledge about elementary reactions in the catalytic reduction of NO_x in exhaust gases has been further increased via lab-scale experimental work and molecular modelling activities.

Electrochemistry Laboratory

Research of the Laboratory is dedicated to innovative solutions in the fields of electrochemical conversion and storage devices, encompassing fuel cells, batteries, supercapacitors, electrolysis, electrocatalysis, and modern methods for electrochemical materials development and interface analysis. Progress is closely related to a better understanding of the properties of materials and components used in electrochemical devices.

Electrodes, electrolytes, and structural materials have to undergo comprehensive *ex situ* and *in situ* characterization processes to be optimized with respect to the complex physicochemical functions required in a cell. Advanced materials characterization methods available at PSI's large facilities, e.g. small angle neutron scattering (SANS) and others, become more and more important for our work.

In addition, the development of novel *in situ* characterization methods for fuel cells is of utmost importance, giving insight into the complex phenomena of the charge and mass transfer coupling processes. Local resolution of current density inhomogeneities on a sub-mm scale related to the cell design can now be achieved.

First year of operation of the Competence Center Energy and Mobility

Philipp Dietrich, CCEM; Alexander Wokaun, Research Department General Energy, PSI

In a collaborative approach of institutions both outside and within the ETH domain, the Competence Center Energy and Mobility (CCEM) was started at the beginning of 2006. Its aim is to support larger projects within the field of energy and mobility research, in close cooperation between the academic institutions and industry as well as other funding agencies.

Vision and mission

The vision of the Competence Center Energy and Mobility (CCEM) is a more sustainable energy system, which provides the energy services required for economic growth with strongly reduced primary energy input. The system meets the societal demand for services in an economically affordable and environmentally compatible manner, thereby preserving the Earth's climate. The 2000 Watt society is a metaphor for such a system.

Energy and climate are global issues, and hence the design of the Center takes into account the global, European, and the Swiss dimensions. As a guideline, the problems to be addressed by the Center must excel in their high relevance to sustainability, science, and industry. They are defined in collaboration between the research community and industry. Therefore the projects of the CCEM shall be focussed around the following mission:

- Reducing the CO₂ emissions of the Swiss energy system.

- Enhancing security of supply by decreasing the dependence on imported fossil energy carriers.
- Increasing the use of energy carriers based on renewable primary energy sources.
- Increasing the efficiency of energy use and reducing the polluting emissions of the energy conversion systems.

In order to target a significant impact on society, projects are designed together with stakeholders, and will strengthen the competitiveness of Swiss industry through the development of new and innovative systems, products, and services.

Research projects

In the first year two calls for proposals were organized. The projects listed below are those which are so far supported by the CCEM. They are classified in the areas of transportation, electricity, heat and buildings.

Transportation

Hydrogen-driven municipal vehicle (hy.muve):

Application of a fuel cell system within a municipal vehicle, and socio-economic study on niche market entry.

Next generation exhaust aftertreatment for diesel propulsion systems (NEADS):

The development of components, and integration, of a selective catalytic reduction system with a diesel particulate trap system, for future truck engines.

Dynamic test rig:

A new test rig for truck engines, in particular for dynamic operation testing.

Transition to hydrogen-based transportation:

Assessment of life-cycle emissions, economics and market

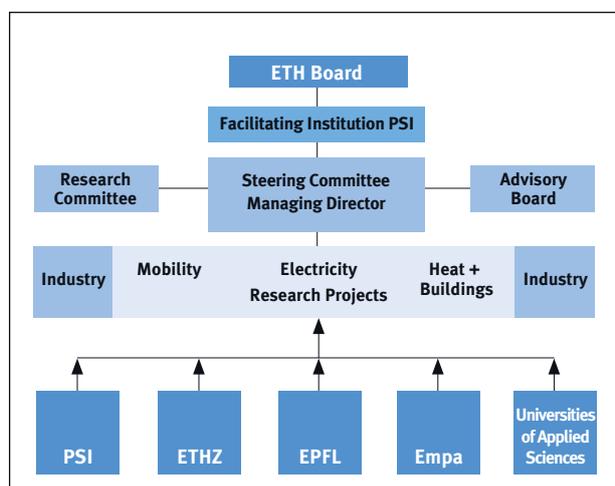


Figure 1: Organization of the CCEM.

dynamics to determine potentials of application of hydrogen as large-scale energy carrier.

Large engine research facility (LERF):

Test facility for large-scale engines (in the MW class) to test new combustion processes in realistic scale, for example as in the case of ship engines.

Clean and efficient large diesel engines (CELaDE):

Development of techniques for in situ measurements on large engines and investigations on high boost turbocharged engine concepts.

Electricity

Computational engineering of multiscale transport in small-scale surface-based energy conversion:

Development of new simulation codes to combine micro- and macro scale phenomena for multi-species transportation and reactions. The application of these codes on a specific application (100 W solid oxide fuel cell).

Platform für high temperature materials:

Installation of specific tools for the investigation of characteristics of high temperature materials, including radiation damage.

Battery replacement using miniaturized solid oxide fuel cell (ONEBAT):

Development of a miniaturized SOFC hybrid power system in the power range of 2–5 W.

Cost-efficient thin film photovoltaics for future electricity generation:

Investigations on the production processes for thin film Si-based photovoltaic cells and investigations of organic-based PV concepts. Fostering collaboration and exchange between the different groups and methods within Switzerland.

HydroNet – modern methodologies for the design, manufacturing and operation of pumped storage power plants:

Improving new operation concepts for hydropowered power plants including issues of dynamic operation.

Heat and Building

Advanced energy-efficient renovation of buildings:

Investigation of a concept for a more industrialized renovation process, investigation of components for such modules and a 3-D laser-based positioning system to explore the exact information of real buildings. Development of software to evaluate the investment strategy for energy efficient renovation.

Innovative building technologies for the 2000-Watt society: Investigation of modules for passive buildings which can be



Figure 2: **A research focus of CCEM is in building renovation.** (Photo: EMPA)

integrated in new buildings. Within this project, demonstration units shall be realized to spur the dissemination into society.

Organisation and procedures

The CCEM is a competence center of the ETH domain fostering joint projects of the partner-institutions, i.e. the ETH Zurich and ETH Lausanne, the research institutions EMPA and PSI, as well as Universities of Applied Sciences and industry. PSI is the facilitator and it is where the management of the center is located (Figure 1).

To support the quality of the CCEM decisions, the steering committee is supported by a research committee and an advisory board (foreseen).

In the steering committee, all partner institutions and industry are represented. In the research committee, representatives who are in charge of scientific quality assessment at their home academic institutions, are working together to assure highest quality standards of the CCEM projects. The advisory board is still to be formed.

In the proposal review process, the submitted proposals were evaluated within the research committee as well as by external experts. In the first year more than 200 external reviewers have been contacted to support the evaluation of the proposed projects.

Acknowledgements

The support of the ETH domain for running the CCEM and for seed funding of the projects with 10–20% of the project volumes is gratefully acknowledged, as is the support of the Canton Aargau which provides funding to further the collaboration between the ETH domain and the FHNW.

Efficient power production from biomass using high-temperature fuel cells

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The combination of wood gasification and high-temperature fuel cells such as solid oxide fuel cells (SOFC) is a promising approach to reach high electrical efficiencies of up to 50 % in small-scale power plants. This combination is referred to as biomass-integrated gasification fuel cell system (B-IGFC). For the first time tests of the whole system with real wood gas were performed at PSI and the proof of concept was achieved. The B-IGFC system at PSI was operated for more than thirty hours. The SOFC system produced peak power values over 560 W, as compared to 880 W in natural gas operation, and 7.4 kWh of electricity were produced.

Potential of biomass

Stationary heat and power generation by means of solid oxide fuel cells (SOFC) has drawn a lot of interest in the past years. This is due to their capability of directly oxidizing carbon-based fuels with high efficiencies at small scale (CH_4 , CO, etc.) and at a high temperature level.

Biomass has a large potential for renewable electricity generation. The worldwide installed capacity of biomass plants was approximately 34 GW in 2002 and is expected to increase up to approximately 100 GW by 2030, still leaving 94% of the world's biomass potential unused [1]. A highly promising approach in this respect is the combination of biomass gasification with SOFCs. The producer gas (PG) obtained from the biomass gasification consists mostly of hydrogen and carbon monoxide, the rest being carbon dioxide, methane, other hydrocarbon species, nitrogen (in case of air as gasification agent), water and diverse impurities (e.g. tars, alkali salts, sulphur, soot particles etc.). The PG has to be processed in order to meet the fuel gas requirements of the SOFC in question. Only a few experiments using synthetic gas mixtures have been performed to assess the effect of potential pollutants to determine the fuel gas requirements, e.g. [2]. As a consequence, most of the published data is based on conservative assumptions, or derived from natural gas applications, e.g. [3], [4]. Moreover, the PG composition strongly depends on the gasification technology, biomass fuel and gasification agent. This has led to numerous gas processing concepts for B-IGFC systems. From previously performed technical system analysis we concluded that a link-up of an updraft wood gasifier with a SOFC via hot gas processing would be a promising system design. Losses of sensible heat

are minimized as the PG is not cooled down in the gas processing section. During first trials at PSI, the operational behaviour of a PG-fed SOFC was investigated on lab scale. In total over 100 h of operation time with real PG were accumulated [5]. Based on these promising results, a 1 kW SOFC system was coupled with the PSI updraft wood gasifier and first test runs were carried out.

Experimental setup

The updraft wood gasifier at PSI employs air as the gasification agent, which is introduced through the grate, while the wood is introduced at the top of the gasifier. The obtained PG is highly tar-laden. The gasifier and the wood pellet hopper can be operated under pressurized conditions up to 3 bar and allow for 24 hours of unattended operation. Coarse particles



Figure 1: B-IGFC system scale test setup at PSI.

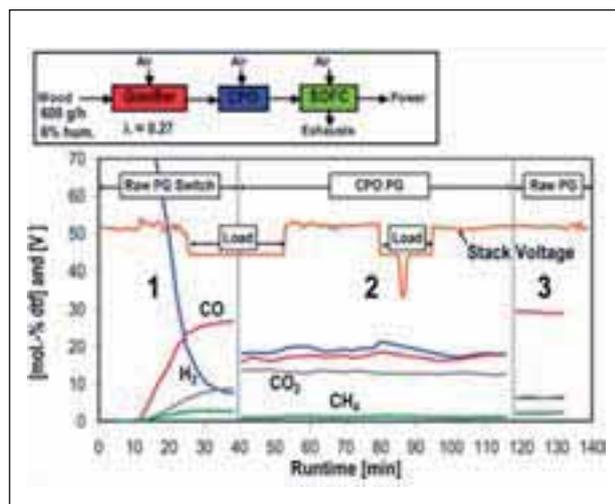


Figure 2: **Stack voltage in open circuit operation and under load conditions. Measured producer gas composition upstream (1) and (3) and downstream (2) of the CPO.**

in the PG are removed in a high temperature cyclone. The highly tar-laden PG is then fed to a catalytic partial oxidation reactor (CPO), where approximately two thirds of the tars originating from the gasification process are catalytically converted to H_2 and CO . A desulphurization unit was integrated to remove hydrogen sulphide (H_2S) and carbonyl sulphide (COS). The employed sorbent is zinc oxide (ZnO). Approximately one-third of the desulphurized, low tar-laden and almost particle-free PG is fed to a 1 kW SOFC system, the rest is flared, see Figure 1.

Results

Figure 2 illustrates the stack voltage and measured PG compositions up- and downstream of the employed CPO during a short test of approximately two hours.

The sections marked 1 and 3 show the composition of the raw PG measured upstream of the CPO, where 1 depicts the measurement during the switch phase from pure hydrogen operation of the SOFC system to PG operation, and 3 gives the measurement at steady-state conditions. By comparing 1 and 3, it can be seen that the raw PG composition obtained from the gasifier was approximately constant during the experiment. The tar and water loads of the raw PG were calculated to be around $120\text{ g}/\text{m}_n^3$ each. It has to be pointed out that the PG was processed via CPO prior to being fed to the SOFC throughout the whole experiment. The PG composition was also measured downstream of the CPO (2). It was found that a significant amount of the tar load in the PG was converted in the CPO. The CPO showed good performance over the duration of the experiment with no signs of degradation. The open

circuit voltage of the SOFC remained constant during PG operation. With this setup, continuous experiments lasting up to twelve hours were possible. In total, thirty hours of operation were accumulated. During this period, over 75 m_n^3 of dry wood gas with an average tar load of 40 g per m_n^3 and an average water load of 120 g per m_n^3 were fed to the SOFC system. The pressure drop over the SOFC did not increase. This indicates that no important carbon deposits occurred. The SOFC system produced peak power values over 560 W as compared to 880 W in natural gas operation. 7.4 kWh of electricity were produced. The current voltage curves before and after PG operation showed minor degradation.

Conclusions – future power generation

The performed pilot tests have proven the PSI concept for B-IGFC systems. Although the experiments were short for industrial standards, the results indicate that the employed simple gas processing system was effective enough for a stable operation of a SOFC. This supports the expectation that the technology as a whole can be made less complex than generally assumed and therefore compete with established systems. B-IGFC systems could play an important role in future power generation from renewables.

Acknowledgements

We thank our industrial partner for providing their 1 kW-SOFC system, the AXPO Naturstrom Förderfonds for their financial support and the Technikteam of our laboratory for their efforts to realize this test setup.

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The rapid quench – a challenge for the thermochemical ZnO/Zn cycle

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Separation of gaseous zinc and oxygen at the exit of a high-temperature solar reactor is crucial for realizing an energy-efficient solar water-splitting thermochemical cycle based on the zinc oxide/zinc redox pair. Separation by rapidly quenching the gaseous products is a promising strategy requiring control of complex physical and chemical processes such as homogeneous nucleation of zinc vapour and oxidation of zinc droplets. The methodologies and tools for optimizing quench units for high zinc yield are described below.

The two-step water-splitting thermochemical cycle via zinc oxide/zinc (ZnO/Zn) redox pair, depicted in Figure 1, has been identified as a promising path for solar hydrogen production because of its potential for reaching high-energy conversion efficiencies and consequently, the prospect of economic competitiveness [1].

Among many technical challenges, the separation of gaseous zinc and oxygen at the exit of the solar reactor is of prime importance for realizing the thermal dissociation of ZnO with a high zinc yield. Separation by a rapid quench of the gaseous products is a viable strategy if process conditions can be identified that sufficiently favour nucleation and condensation of zinc against the re-oxidation of the created droplets or crystallites.

Modelling of the quench process

The complex physical and chemical processes occurring at the rapid quench are investigated by modelling the prevailing

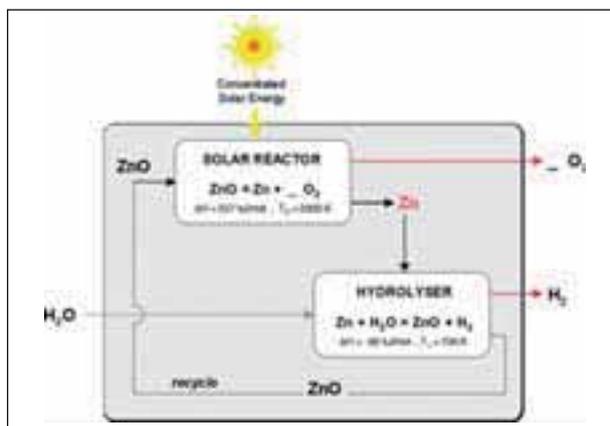


Figure 1: **The thermochemical ZnO/Zn cycle.**

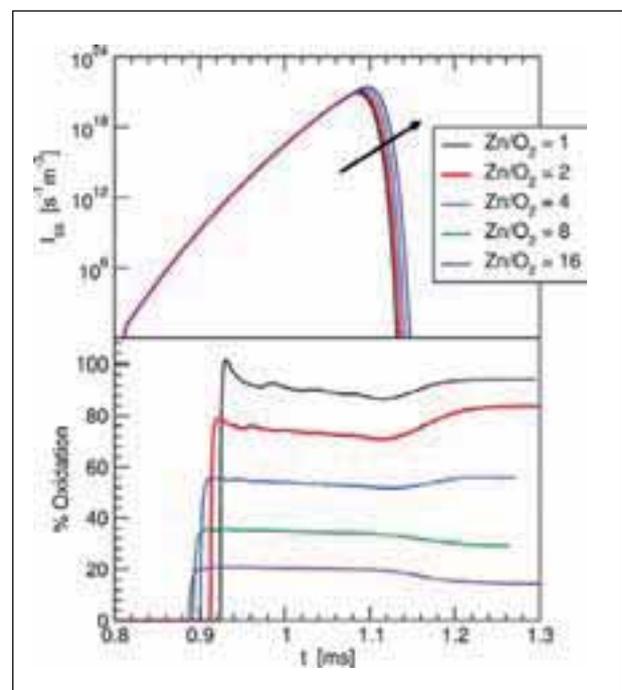


Figure 2: **The nucleation rate I_{ss} and the oxidation degree of a Zn/ O_2 mixture in function of the initial partial pressure ratio p_{Zn}/p_{O_2} and of time.**

traits of the physical situation mainly characterized by the formation of zinc droplets and of ZnO. The latter is not a gas phase reaction but occurs only on solid or liquid surfaces, i.e. at walls or on the created droplets.

The following computational model comprises four fundamental processes: (1) homogeneous nucleation of zinc vapour, (2) condensation of zinc atoms on a zinc surface, (3) reaction of oxygen at a zinc surface forming a surface layer of ZnO, (4) addition of zinc atoms on top of a ZnO-layer. The four proc-

esses are driven by imposing a rapidly decreasing temperature profile onto the system typically starting with a slightly undersaturated gas mixture. Appropriate nucleation and condensation rates must be given. Mass balances account for the zinc and oxygen depletion of the gas. The model delivers the number of formed clusters as a function of their zinc and oxygen contents and of time. Subsequently, the partial pressures of zinc and oxygen, the total free zinc and oxidized surfaces, and the degree of oxidation can be derived. As an example, Figure 2 shows the nucleation rate I_{ss} and the oxidation degree for different initial fractions of the zinc and oxygen content, $Zn/O_2 = 2$ denoting the stoichiometric mixture. Sticking probabilities of 0.1 are chosen for the processes (2) to (4). Initial values are $T = 1000$ K and $p_{Zn} = 11$ kPa corresponding to an initial saturation of 0.96. The temperature decrease is constant at -10^5 K/s.

While the nucleation rate I_{ss} depends only on the zinc saturation, the degree of oxidation markedly depends on p_{O_2} : the highest oxidation degrees occur during nucleation. After 1.1 ms, the oxidation degree continues to decrease if the oxygen has been consumed. It increases again if there is still some oxygen in the gas phase.

Empirical investigation of the quench

The sticking probabilities for the processes (2) to (4) are the basic model parameters. They are arbitrarily chosen for the preliminary model calculations presented but will be determined, finally, from comparison with experimental data. Three experimental devices are being employed. Zinc nucleation and condensation is currently studied with an oxygen-free experiment where a mixture of nitrogen and zinc vapour is ex-

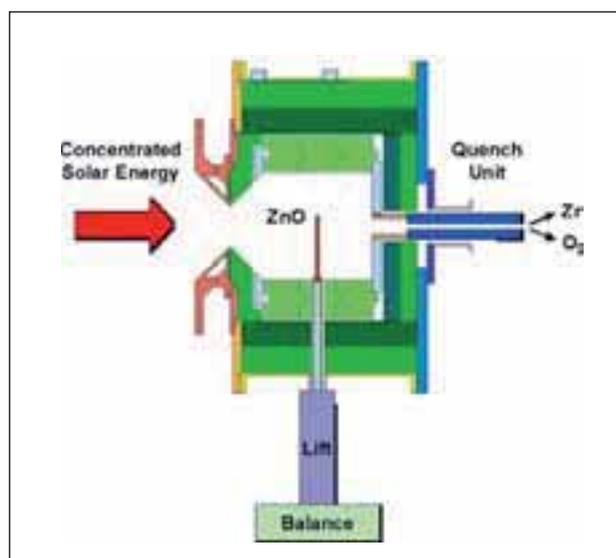


Figure 3: Schematic of the solar thermal gravimeter.

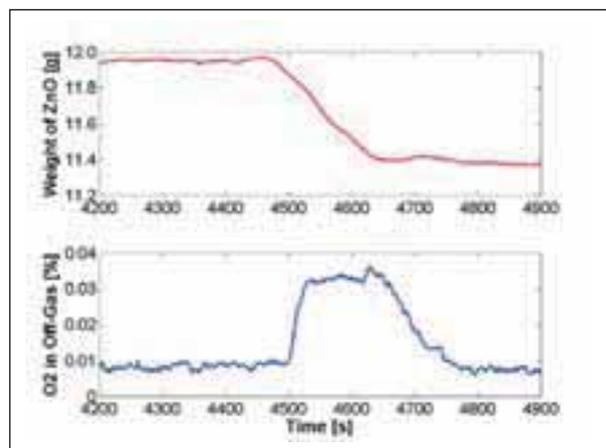


Figure 4: Results with Solar TG: weight loss of ZnO due to dissociation and O_2 content in the off-gas.

panded through a Laval nozzle [2]. The quenching of $Zn(g)-O_2$ mixtures is tested with the two set-ups ‘quench tower’ and ‘solar TG’ (solar thermal gravimeter).

A schematic of the solar TG is shown in Figure 3. It consists of a solar cavity reactor into which a ZnO sample can be introduced with a lift mounted on a balance. During an experimental run, the reactor is first heated to the desired temperature and maintained under isothermal conditions. A ZnO sample is then inserted and directly exposed to high-flux solar irradiation. The product gases of its dissociation, diluted in argon (Ar), are directed to the quench unit where they are mixed with cold Ar. Particles formed are then filtered out for further analysis. The efficiency of the quench is determined from the weight loss of ZnO recorded and the amount of O_2 measured in the off-gas.

A typical result is shown in Figure 4. After a preheating time of about 4400 s, the ZnO sample is lifted into the cavity and starts to dissociate. The oxygen content in the off-gas increases, proving a partial suppression of the zinc re-oxidation. A zinc recovery up to 30% has been obtained in preliminary exploratory runs. Validation of the computational model with the experimental data will allow the determination of the optimal conditions for maximizing the zinc yield.

Acknowledgements

Financial support by the Swiss Federal Office of Energy (BFE) is gratefully acknowledged.

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On catalytic micro reactors for small-scale power generation

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Portable power generation devices (<100 W) using hydrocarbon fuels have received increased attention due to their possible superior power density compared to batteries. Small-scale catalytic combustors (of the order of a few cm³ volume) are well-suited for providing power to the thermodynamic cycle of such devices (such as small-scale gas turbines) due to their superior thermal and combustion stability under the associated large surface-to-volume ratios present at the microscale. The performance of these combustors is determined by the heat transfer characteristics of the material used.

Introduction

Small-scale thermochemical devices driven by hydrocarbon-fuelled combustors have received increased attention in portable power generation applications due to their superior power density compared to state of the art Li ion batteries [1]. Catalytic processes, in particular, are well suited for small-scale hydrocarbon combustion due to the associated large surface-to-volume ratios. A recent initiative at ETHZ [2] explores gas turbine-based mesoscale (up to 1 kW_e) power generation systems (see Figure 1), with PSI being involved in the combustor development.

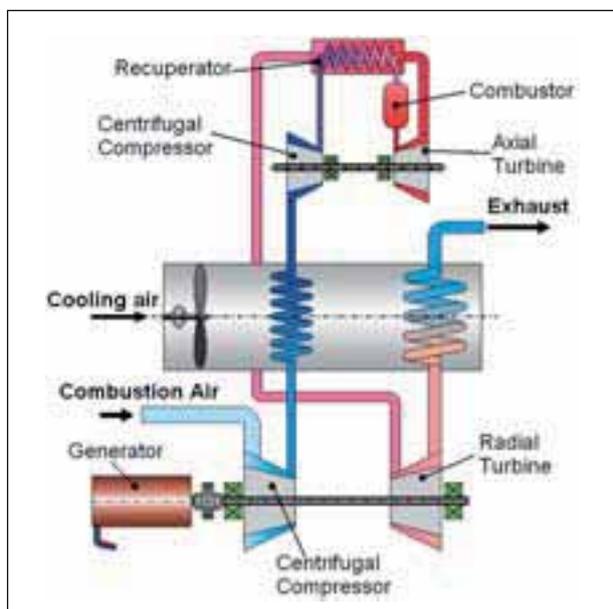


Figure 1: Swiss initiative for mesoscale gas turbine power generator [2].

The present work presents first a theoretical and then an applied numerical investigation of combustion stability maps and performance characteristics in such systems.

Fundamental studies on catalytic reactors

In the former front, the stability limits of methane fuelled catalytic microreactors (Pt coated) have been delineated in a 1-mm-gap channel at pressures of 1 and 5 bar (the latter being the maximum foreseeable pressure in the reactor of Figure 1). Heat losses from the external wall channel surfaces to the surroundings have been modelled via a heat transfer co-

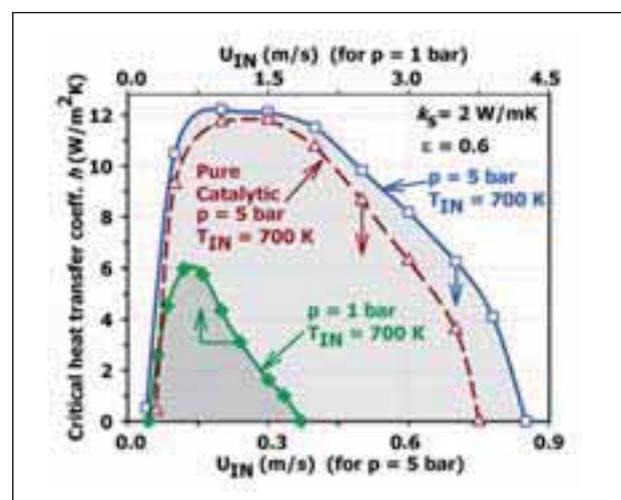


Figure 2: Stability diagrams for critical external heat transfer coefficient vs inlet velocity for $T_{IN} = 700\text{ K}$, $p = 5\text{ bar}$ (squares: catalytic and gas chemistry, triangles: only catalytic chemistry) and $p = 1\text{ bar}$ (diamonds). Shaded areas show the stable regimes.

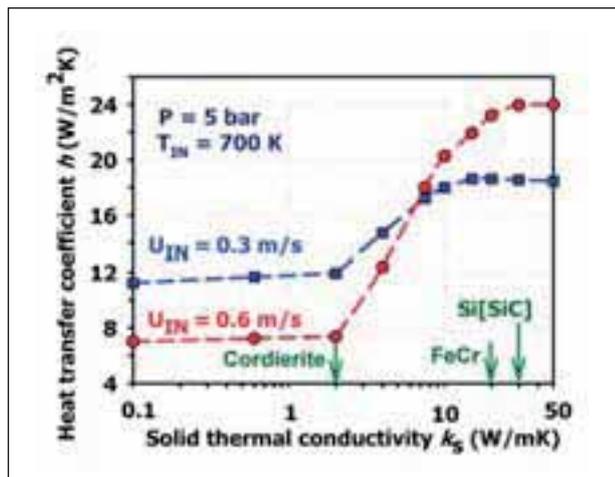


Figure 3: Critical heat transfer coefficient versus solid thermal conductivity.

efficient h . This parameter, along with the wall thermal conductivity and the inlet velocity, played a profound role on the stability limits of the reactor. It was shown [3] that gas phase chemistry extended the low velocity extinction limits due to the establishment of strong flames and to an even greater degree the high velocity blow-out limits due to the heat release originating primarily from the incomplete homogeneous oxidation of methane. When considering the same mass throughput, the stable combustion envelope at 5 bar was substantially wider than its 1 bar counterpart due to the increased reactivity of both catalytic and gaseous pathways with increasing pressure (see Figure 2). Stable combustion could be sustained with solid thermal conductivities at least as low as 0.1 W/mK, while the stability limits reached their larger extent between 15 and 30 W/mK, a range that encompasses many practical metallic compounds (Figure 3).

Propane-fuelled catalytic combustor

On the applied side, a Pt-coated, propane-fuelled catalytic monolithic reactor has been investigated for portable turbine-based power generation, its design being part of the initiative of Figure 1. Detailed parametric numerical studies were conducted [4] for two reactor materials (ceramic and metallic), and combustion efficiencies were assessed at different inlet velocities and equivalence ratios. An operating scenario was chosen with a moderate mixture compression at $p = 2.5$ bar, fuel-to-air equivalence ratios up to $\phi = 0.40$ and preheat temperature $T_{IN} = 750$ K (achievable in recuperated mesoscale gas turbine devices). Power output curves and combustion efficiencies have been calculated for different inlet velocities, equivalence ratios, solid thermal conductivities (k_s) and solid

thicknesses (δ). It was shown that, for a given reactor length, metallic materials were more favourable regarding maximum power output and combustion efficiency (Figure 4).

Reactors with high solid thermal conductivity displayed increased fuel conversion at high inlet velocities, due to reduced light-off distances and the larger surfaces exposed to high temperatures compared to reactors with low-wall thermal conductivities. Metallic reactors benefited from more robust construction (thicker solid walls) when operated under fuel-leaner conditions, while ceramic reactors profited only by increased equivalence ratios.

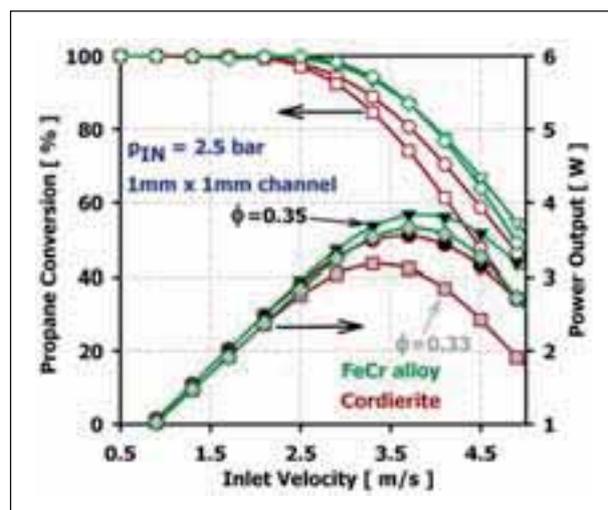


Figure 4: Combustion efficiency and power output curves versus inlet velocity for channel inlet conditions: mixture preheat 750 K, pressure 2.5 bar. Gray symbols: $\phi = 0.33$, black: $\phi = 0.35$. Triangles: $k_s = 14$ W/mK, $\delta = 0.1$ mm. Circles: $k_s = 2$ W/mK, $\delta = 0.1$ mm. Diamonds: $k_s = 14$ W/mK, $\delta = 0.2$ mm. Squares: $k_s = 2$ W/mK, $\delta = 0.2$ mm.

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High-resolution current mapping in fuel cells

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In the search for higher performing and cheaper fuel cells we have developed a novel method for measuring current distributions in polymer electrolyte fuel cells (PEFC). In contrast to all other techniques, it allows for a resolution smaller than the channel/rib scale of a PEFC's flow field for the first time. Current density is obtained by considering the electron-conducting cell components as 2-dimensional shunt resistors, through which the electric current causes a measurable voltage drop. The method is applied for investigating local power losses. Results show that ohmic resistances and transport limitations in the porous media limit current generation on this sub-millimeter scale.

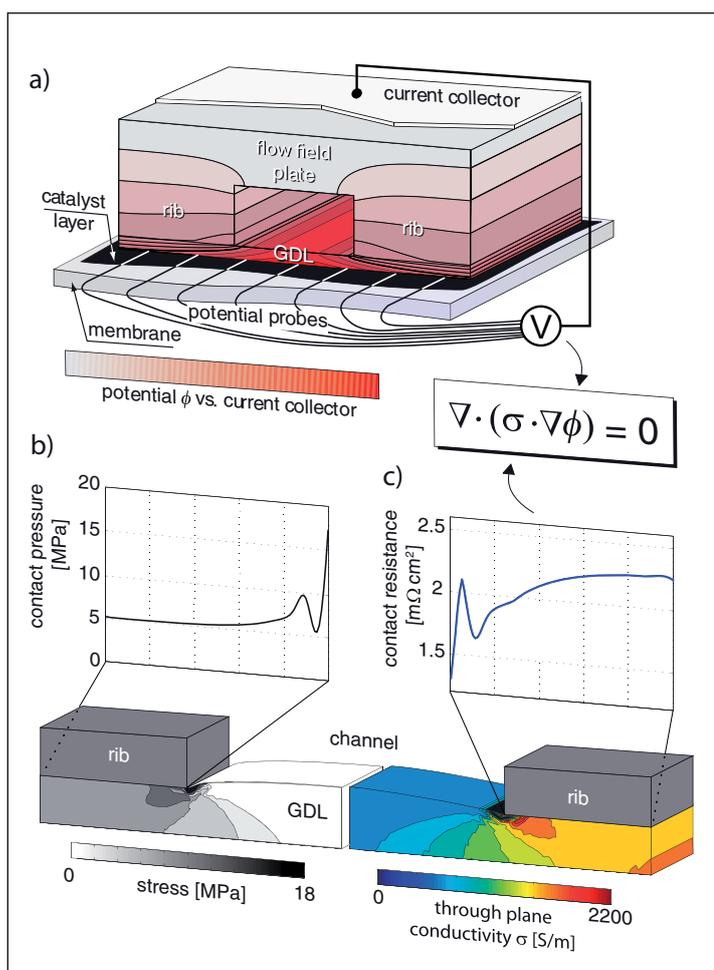


Figure 1: a) Schematic of the potential measurement. b) Stress distribution in a compressed GDL. c) Conductivity distribution in a compressed GDL, factors that need to be investigated for obtaining local current density across channel and rib.

In today's PEFCs, the current density distribution on all scales is of high interest for the optimization of cell structures with respect to power density, which is associated with performance and costs. On the sub-millimeter scale, the current density is inhomogeneous over flow field ribs and gas channels. Until now, only simulations have been available for describing this local current generation. Experimental data has been restricted to the correlation of flow-field structures to integral cell performance.

Consequently, a novel method for measuring the current density distribution on a scale smaller than the channel and rib spacing has been developed [1,2].

Measurement principle

The measurement principle is based on the idea of considering the electron conductors of a fuel cell's electrode as 2-dimensional shunt resistors (i.e. anisotropic in the directions perpendicular to the channel and the membrane). The drop of the potential ϕ between catalytic layer (CL) and current collector has to be measured with a resolution of several points per channel and rib. For this purpose, potential probes in the form of fine wires (10 μm) are inserted along the channel at the interface of CL and gas diffusion layer (GDL), as shown in Figure 1a.

The current density in GDL and flow-field plate is then obtained from the solution of Laplace's equation with the potentials at current collector and CL as boundary conditions. As a quality criterion, the mean value of calculated current is compared to the load applied to the cell.

As current density is obtained indirectly from the ohmic drop, the precise knowledge of all resistances involved is of prime importance. In particular, the anisotropic GDL bulk conductivity as well as the contact resistance between GDL and rib strongly depend on clamping pressure and therefore require careful consideration.

The spatial distribution of the resistivity is determined by the distribution of the compressive stress, which differs strongly across channel and rib. Consequently, structural mechanics calculations are applied to obtain the local pressure. Figure 1b shows the dispersion of contact pressure across the flow field land and the resulting stress distribution in the GDL bulk. The corresponding GDL conductivity σ and contact resistance is illustrated likewise in Figure 1c.

Insights gained

Experimental results show that the high-resolution current distribution is mainly governed by two effects: ohmic resistance and oxygen mass transport. At low load, the higher fraction of current is generated under the rib areas. This is caused by the lower ohmic resistance at this location, which promotes local current production. With increasing integral current, however, the current maximum is gradually shifting to the channel area. Due to the longer diffusion pathways under the rib, local reactant activity is reduced even when the cell is operated on pure oxygen (see Figure 2a). The advantage of lower resistance under the rib is now offset by mass transport limitations. The 3-D plot also shows a small current peak at the rib edge, where oxidant transport is favoured and contact- and GDL resistance are low.

The mass transport limitation becomes more pronounced when the oxygen partial pressure is reduced (as is the case in areas near the air outlet in real applications). Figure 2b illustrates that even at medium current densities a distinct current peak develops under the middle of the channel when lowering the oxygen partial pressure. The 3-D plot shows the evolution of the current partition along a channel when the oxygen fraction is reduced from 1 to 0.05.

Figure 3 shows local current-voltage curves for a cell operated on 10 % O_2 . Current generation under the rib becomes inhibited before limitations are clearly observed in the integral characteristic. Hence, the new measurement technique allows for assessing current losses due to local limitations. As a consequence, improving PEFC performance and durability becomes feasible by geometric and material adaptations on the sub-mm scale.

Acknowledgements

The financial support of the Swiss Federal Office of Energy (BfE) is gratefully acknowledged.

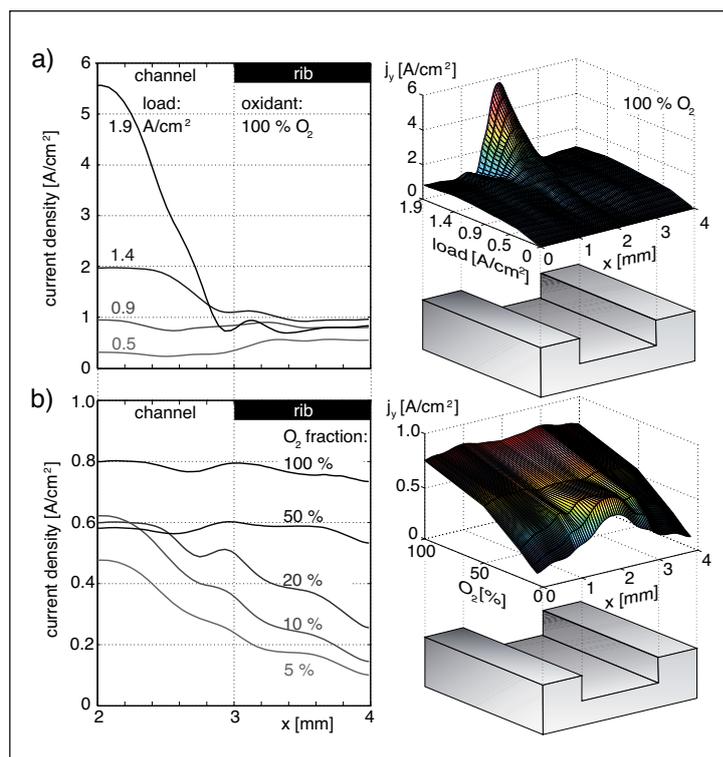


Figure 2: **a) Evolution of the local current distribution with growing current for a cell operated on dry oxygen. b) Comparison of current distributions for decreasing oxygen fractions at 0.5 V cell voltage, dry conditions.**

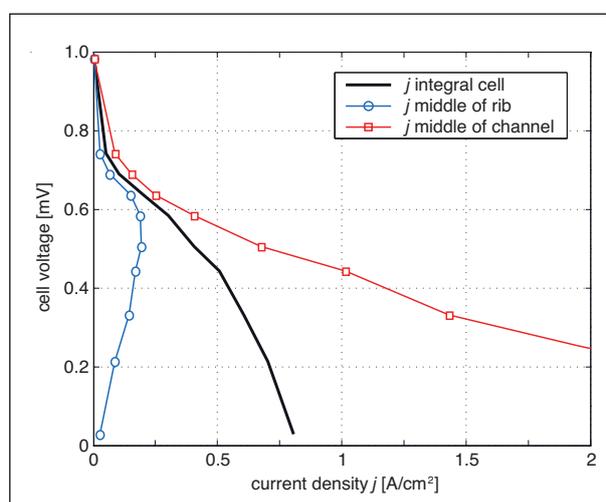


Figure 3: **Local polarization curves for a cell operated on 10 % O_2 in N_2 under dry conditions.**

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Materials research for polymer electrolyte fuel cells

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Polymer electrolyte fuel cells (PEFCs) are electrochemical power sources with high efficiency and therefore could have many applications. However, several challenges such as cost, performance and longevity must be solved before this technology can be brought to the market. The interplay of various materials is necessary for optimal functioning of the cell. Hence, research in different areas of cell materials, for example proton-conducting polymer membranes and electrocatalysts, is of paramount importance for the further improvement of this technology.

The technology of polymer electrolyte fuel cells (PEFCs) has been demonstrated in mobile, stationary, and portable applications. Major challenges still remain concerning cost, power output, and longevity. Materials properties also determine the design and window of operation for the respective fuel cell system. Hence the need for improved materials and, additionally, a better understanding of structure – property relationships require further progress in various areas of materials research, such as polymer chemistry, electrocatalysis and solid-state chemistry.

Proton-conducting membranes

For several years, our laboratory has been involved in the development of proton-conducting membranes, suitable for use as solid polymer electrolyte, on the basis of the radiation grafting process [1]. Progress has been achieved in the up-scaling of the membrane preparation process for poly(tetrafluoroethylene-co-hexafluoro-propylene) (FEP) based membranes to some hundreds of cm², suitable for cell areas of technical interest. An alternative base polymer film, poly(ethylene-*alt*-tetrafluoroethylene) (ETFE), has been evaluated and the grafting process optimized, in particular with respect to the cross-linker content of divinylbenzene, DVB. (Figure 1) [2]. Fuel cell performance similar to our standard membrane based on an FEP-film and the commercial standard membrane of the Nafion 112 type can now be achieved.

For the further optimization of these types of radiation-grafted membranes, we study the influence of alternative monomers as graft components. The combination of α -methylstyrene (AMS) and methacrylonitrile (MAN) allows interesting improvements of stability as compared to the conventional grafted monomer styrene [3]. As in the case of styrene as grafted monomer, also with these monomers the optimization of cross-linking plays an important role in fuel cell performance.

Post-mortem analysis of membranes provides conclusions with respect to local influences of the cell design onto the

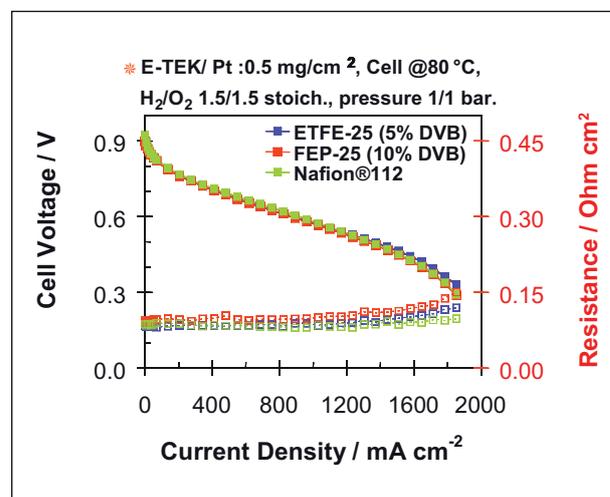


Figure 1: Current-voltage curve of optimized membrane based on 25 µm thick poly(ethylene-*alt*-tetrafluoroethylene) ETFE films.

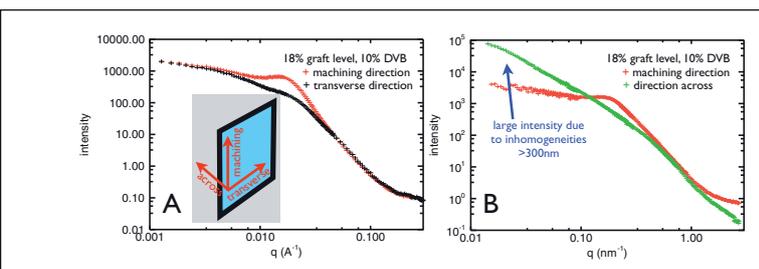


Figure 2: **Characterization of radiation grafted films in dependence of film orientation by SANS. The hump at $q=0.015 \text{ \AA}^{-1}$ is due to a typical distance between domains, which is most pronounced along the machining direction.**

stability of fuel cell components, such as the membrane electrolyte. The local analysis, as defined by the flow-field pattern of the bipolar plate, yields important information about how degradation of membranes occurs in dependence of fuel cell conditions [4].

An understanding of the microstructure of these ion-conducting polymers, in particular in dependence of the preparation conditions, will lead to a further improvement in tailoring the properties to the requirements of the fuel cell. Small angle neutron scattering (SANS) has been applied to study the nanostructure of films and membranes in dependence of the preparation conditions. The obtained results demonstrate an anisotropic morphology of the grafted films, which, as a consequence, lead to anisotropic properties, such as conductivity and toughness [5].

Electrocatalysts

Platinum or platinum alloys are still the standard electrocatalyst in PEMFCs. A further reduction in platinum metal content without a penalty in performance is one of the major challenges in the development of this technology. We applied a co-sputtering process of platinum and carbon to prepare catalytically active areas with a platinum content lower than the one of commercial electrodes, and were able to demonstrate similar fuel cell performance [6]. Although this process is still far from being optimized it is a step closer to the required cost targets.

An understanding of the fundamental electrochemistry of platinum is also necessary to optimize the interface between the ionomer membrane and the electrocatalyst. During the preparation of stable polycrystalline platinum electrodes in contact to an aqueous electrolyte we came across a novel platinum morphology, which exhibits an unusual inertness against electrolyte impurities [7].

Micro fuel cells

Micro fuel cells could be used as battery substitutes in small power supplies. We have developed a microstructuring process for glassy carbon, a material suitable as separator plate for these applications. The novel cell concept utilizes these plates directly in combination with a catalyzed coated membrane (CCM), without gas diffusion layers. Geometric power densities of several 100 mW/cm^2 have been demonstrated [8,9].

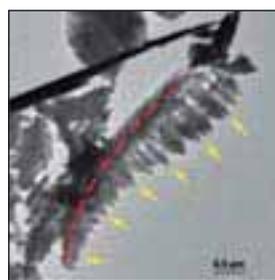


Figure 3: **TEM micrograph of 'feathered platinum', a novel platinum surface morphology.**

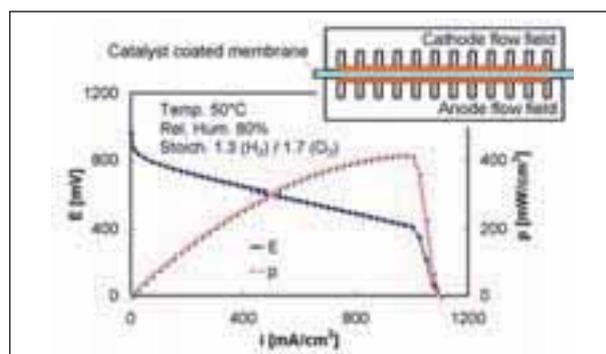


Figure 4: **Current-voltage and current-power curves of a 1 cm^2 micro-structured fuel cell.**

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Monte Carlo analyses relevant to Swiss reactors

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Taking advantage of the availability of high-performance computing resources, Monte Carlo simulation of neutron transport has become the standard approach for certain high-fidelity, safety-related analyses of nuclear power plants (NPPs). Examples are the assessment of criticality safety and fast-neutron fluence of the reactor pressure vessels (RPVs). Both applications require neutron transport calculations to be undertaken for heterogeneous and geometrically complex configurations, with high importance being placed on the modelling of strong neutron flux gradients, scattering anisotropy, etc., for which deterministic methods may involve undesirable approximations. Use of the Monte Carlo code MCNPX for such analyses in the context of the Swiss NPPs is outlined here.

In order to develop capabilities for a comprehensive safety analysis of the Swiss NPPs, a set of state-of-the-art codes, calculational models, data sets and appropriate data transfer tools is being maintained within the project STARS (Safety research related to Transient Analysis of the Reactors in Switzerland).

The Monte Carlo (MC) code MCNPX and general-purpose, point-wise neutron data libraries are employed in the project for those tasks for which the stochastic simulation of neutron transport is particularly advantageous, as well as for calculational benchmarking of deterministic codes. Among ongoing activities, the major tasks that are presently considered to require a MC solution are: (1) criticality safety evaluations (CSEs), including burn-up credit (BUC) analysis [1]; and (2) analysis of the fast neutron fluence (FNF) for light water reactor (LWR) RPVs and internals [2].

Criticality safety evaluations

The purpose of CSEs is to ensure the subcriticality of a system or process under considerations of both normal and (credible) abnormal conditions, taking into account the uncertainties associated with the methodology in use (code, nuclear data, etc). When the CSE is performed in terms of the effective neutron multiplication factor, k_{eff} , the standard approach for evaluating the criteria to establish subcriticality is based on a statistical analysis of the calculational results obtained for a representative set of relevant critical benchmark experiments. Such studies, using MCNPX and point-wise neutron

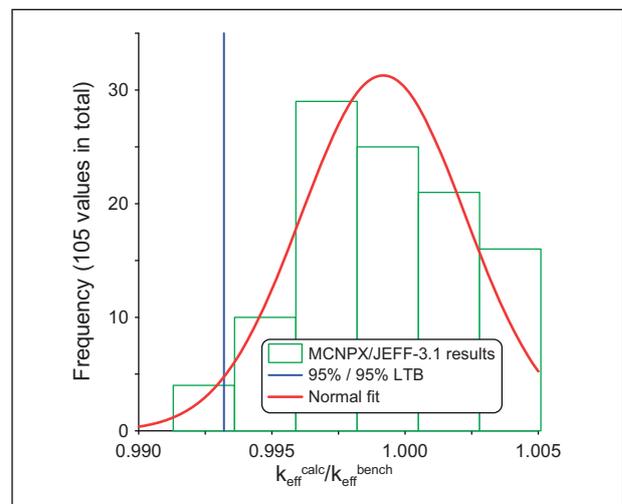


Figure 1: Statistical analysis of calculated-to-experiment k_{eff} values.

data libraries, are currently underway [1], with the objective of upgrading the methodology for the analysis of Swiss storage configurations for discharged LWR fuel assemblies. Consequently, suitable benchmarks from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* have been used as part of the validation process.

An example of the statistical analysis of MCNPX-based calculational results is given in Figure 1. Here, for k_{eff} predictions, the estimated statistical lower tolerance bound (LTB) is shown for specific population proportion/confidence values. The information is needed for the definition of the minimum allowable level of subcriticality in the context of practical CSE applications.

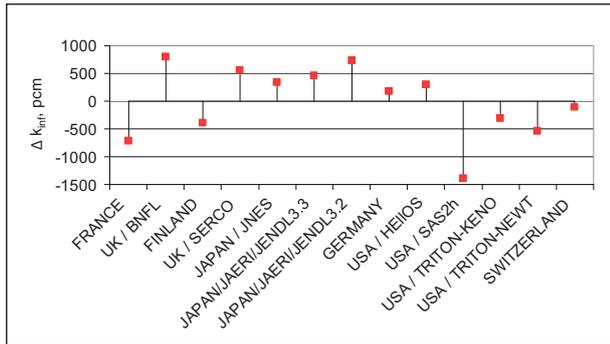


Figure 2: Evaluated results for BUC-IID benchmark.

Studies related to burn-up credit

Taking credit for fuel burn-up of discharged fuel assemblies enables significant cost optimizations for the storage and transportation of spent fuel to be made. Ongoing studies aimed at assessing MC-based computational accuracies in this context, necessary for BUC implementation into CSE methodology. As an example, results of participation in the OECD/NEA BUC calculational benchmark for PWR-UO₂ fuel assembly burn-up and criticality calculations [3] are presented in Figure 2. The value shown, for each participant, is the average deviation (for the 23 cases calculated) of the infinite neutron multiplication factors k_{inf} from the mean values calculated from the submissions by all participants. The PSI (Switzerland) results, obtained with the MONTEBURNS2.0/MCNPX2.4.0/ORIGIN2.1 code system in conjunction with the related data libraries, correspond very closely to the overall mean value.

Fast neutron fluence analysis

Radiation-induced damage in metals, which may be approximated as a function of the FNF, is an important safety-related factor influencing plant lifetime. A novel methodology for accurate modelling of the FNF accumulated in a LWR RPV has been developed and validated in support of the ageing assessment of Swiss NPPs [2]. The methodology is based on the transfer of deterministic CASMO-4/SIMULATE-3 core-follow results (power distribution, fuel compositions), representing the actual reactor operational history, into a three-dimensional volumetric (pin-by-pin) fixed neutron source for ex-core neutron transport simulations using MCNPX.

Appropriate qualification of a methodology for FNF calculations should include comparisons with measurements from operating reactors. To this purpose, ‘scraping test’ data from the RPV of a Swiss NPP have been used as a source of validation for the entire sequence of steps in the FNF analysis. The

computed FNF values, obtained using the currently developed CASMO-4/SIMULATE-3/MCNPX calculation scheme, are compared against the estimates based on activity measurements of the scraping samples in Figure 3. The present calculational results lie within $\pm 5\%$ of the reference values, i.e. well with the declared experimental uncertainty of $\pm 10\%$, and can be considered to be very satisfactory.

Conclusions

As a result of the considerable advance in computing capabilities, and the quality of neutron data (but also as a result of increased safety demands), there is a global trend to intensify the usage of MC codes in neutron transport calculations. The development of current R&D activities at PSI exemplifies this trend. In particular, appropriate application of the MCNPX code within the STARS project has made it possible to achieve a significant enhancement of accuracy for several different types of NPP-relevant analyses, as illustrated by the examples given here.

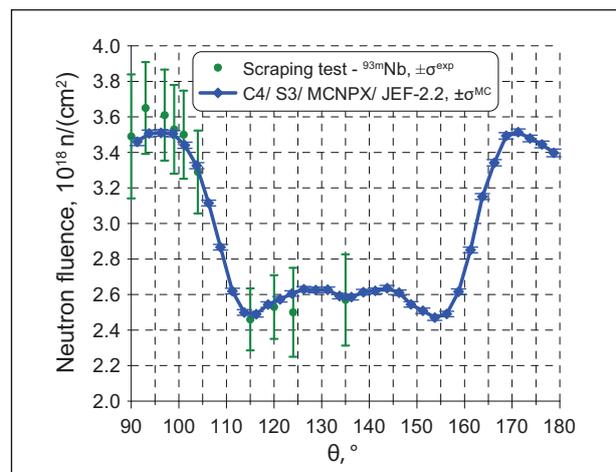


Figure 3: FNF azimuthal distribution over RPV inner surface at core mid-height after 10 reactor cycles.

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Reactor containment studies in the PANDA facility

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The phenomena governing light water reactor (LWR) containment response for certain postulated accident scenarios, include gas (air, hydrogen, steam) stratification in the containment, gas distribution between containment compartments, wall condensation and hydrogen accumulation. The PANDA facility at PSI has been used in the framework of the OECD/SETH project. The test campaign was aimed at producing a database suitable for assessing the capability of codes based on both lumped-parameter approximations and 3D modelling to predict key physical phenomena relevant to LWR safety. The results of one SETH test and its analysis using the GOTH-IC code are described here.

Phenomena such as gas stratification in a LWR containment, gas transport between containment compartments, wall condensation and hydrogen accumulation have been identified as high-ranking phenomena playing an important role in issues directly related to the safety of both current LWRs and future reactor systems. These phenomena may be driven by buoyant, high-momentum jets or low-momentum plumes.

The OECD/SETH project, directly financed by 15 countries, had as its main objective the creation of an experimental database relating to physical phenomena relevant for LWR containment safety analysis. Data have been collected from an extensive programme of 24 experiments carried out in the PANDA facil-

ity. The investigations included three series of tests characterized by wall plumes, free plumes and horizontal jets, respectively. For each test, a combination of two gases has been used: i.e. steam/air or helium/steam (helium is used as a simulant for hydrogen, which would be released during a severe accident). In addition, one plume test has been performed using three gases: air, steam and helium.

The PANDA facility enables the experiments to be performed at a scale approaching the dimensions of actual containment compartments. The unique experimental database thus created is currently being used to assess the capabilities of 3D codes and lumped-parameter (LP) codes to predict phenomena relevant to LWR containment safety.

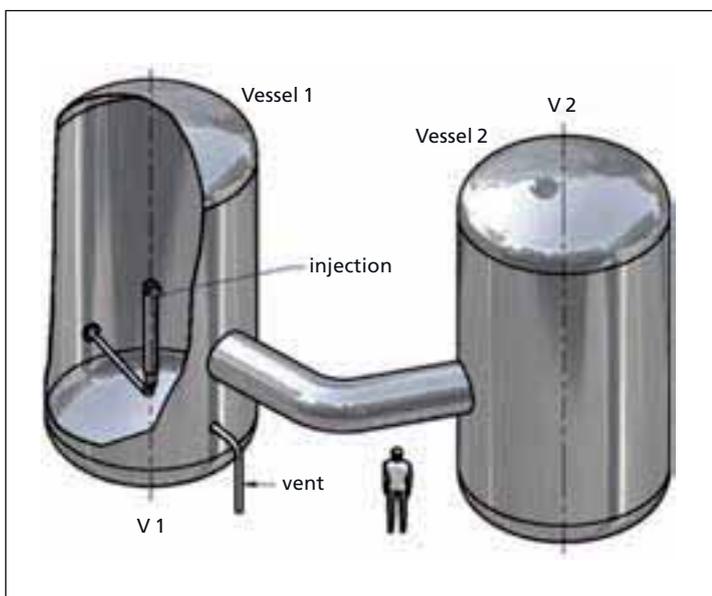


Figure 1: Schematic of the two vessels and IP.

The PANDA facility

PANDA is a unique, large-scale, thermal-hydraulics test facility, designed and used for investigating integral containment system behaviour of Generation III (i.e. near-future) LWR designs (specifically SBWR, ESBWR and SWR1000) under accident conditions, and for the study of 3D phenomena relevant to LWR containments. PANDA has a modular structure, consisting of cylindrical pressure vessels, water pools and auxiliary systems. The total height of the facility is 25 m, and the design operating conditions are 10 bar and 200 °C. Two PANDA vessels have been used for the SETH tests, configured to represent typical compartments in a LWR containment. Each vessel has a diameter of 4 m and height 8 m. The vessels are joined by an interconnecting pipe (IP) of 1 m diameter (Figure 1). The total volume (vessels and IP) is 183 m³.

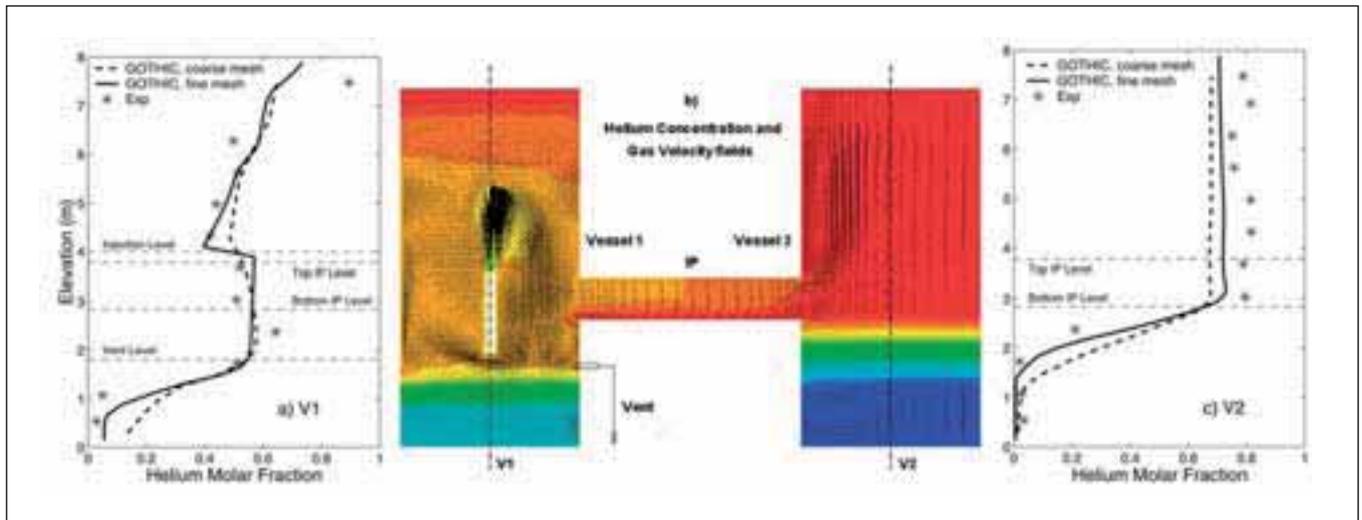


Figure 2: A comparison of GOTHIC predictions and measurements at around 4000 s.

Three-gases plume test

The three gases plume test is composed of two phases, of approximately 2 hours each. During the first phase, a postulated accident with release of steam and hydrogen is simulated (the hydrogen would derive from a zircaloy-water reaction of the fuel cladding due to overheating). In PANDA, the event is represented by a mixture of steam and helium injected into Vessel 1 (Figure 1). The nozzle of the injection pipe is located at mid-height along the central axis of the vessel; both Vessel 1 and Vessel 2 are initially filled with air. During the second phase, only steam is injected (the scenario to be addressed occurs after the zircaloy-water reaction is exhausted).

The evolution of the fluid density in the two vessels, resulting from gas injection, transport and steam condensation, controls the flow patterns, the mixing and stratification. The phenomena are very complex, and involve: free rising plumes, interaction of large-scale flow structures, the change from a buoyant injection phase to a negatively buoyant plume in Vessel 1, flow reversal in the IP, and changes in recirculation patterns, multi-layer stratification and stratification erosion in Vessel 2. Among this multitude of phenomena, those occurring around 4000 s into the transient are presented here, to illustrate how the data collected can be used for code validation, show here in regard to the GOTHIC code [2].

GOTHIC code

This is an advanced containment code which permits the 3D representation of volumes using a Cartesian mesh system. For this study, a coarse mesh consisting of 3250 cells has been used, as well as a finer one of 20'000 cells.

Figure 2b shows the superimposed gas concentration and velocity fields (calculated by GOTHIC with the finer mesh) in a vertical plane through the axes of the two vessels and the IP. It can be seen that the upwards propagation of the steam-helium mixture injected into Vessel 1, which initially rose to the top of the vessel due to buoyancy, is now constrained by the stable stratification created by steam condensation in the dome, and the associated increase in light-gas (helium) concentration. Counter-current flow conditions prevail in the IP, driven by small density differences between the two vessels. The flow pattern in Vessel 2 is characterized by a rising, helium-rich plume. The temperature and gas concentration measurements, taken at several locations in the containment compartments, are consistent with code predictions: calculated and measured vertical helium distributions along the central axis of the two vessels are shown in Figures 2a and 2c. The observed discrepancies are probably due to too little condensation being predicted by the code. Overall, the results obtained with GOTHIC for the entire test indicate that transients characterized by complex evolution of the density differences between compartments remains a challenging task, even for codes those with 3D capabilities. Further code-validation activities are underway, and also foreseen in the second phase of the project (SETH-2).

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Multi-scale modelling: a tool for the future

Wolfgang Hoffelner, Maria Samaras, Botond Bako, Roberto Iglesias, Annick Froideval, Jiachao Chen, Manuel Pouchon, *High Temperature Materials Project, Laboratory for Materials Behaviour, PSI*

The choice of suitable materials and the assessment of long-term material damage are key issues needing to be addressed for the safe and reliable performance of nuclear power plants. Operating conditions of a high-temperature, irradiating and corrosive environment degrade the material properties, posing the risk of very expensive, or even catastrophic, plant damage. Multi-scale modelling of materials is a promising tool to bring new insights into the understanding of basic structural behaviour, and thereby avoid such events.

Equipment operating within extreme environments is usually subject to various conditions leading to damage and ageing of the materials of which it is composed. In order to ensure safe operation of plant components, it is necessary to anticipate such degradation. In applications where the components are easily accessible, and for which typical maintenance intervals are short (e.g. in the automotive industry), or where non-destructive evaluation is easily performed during service, the investigation of components taken out of service prematurely, or where experience has been gained by failure, all help to improve the reliability of the design.

This approach to design optimization fails for long-term applications (50 years or more), and for components which cannot be exchanged (e.g. pressure vessels).

For long term application, Figure 1 schematically illustrates the accepted design procedures. Once the geometry of a component has been defined, the stresses and strains to which

it is subjected are determined by finite-element (FE) calculations. These calculations rely on knowing the precise material properties (determined in the laboratory), and material laws (constitutive equations). Design rules and code standards are then used to evaluate complex loading situations and uncertainties. Modelling can offer physically based insights into the constitutive equations, and can ultimately provide very valuable input into design rules and code standards for damage interactions, as is indicated on the right hand side of Figure 1. This could be an attractive approach for increasing the accuracy of life-time assessments, and consequently the safety of nuclear power plants.

Interactive models

When the term *model* is used in this context, it does not represent the actual FE component, but rather an interactive model, in which the relevant issues – the time and length scales at which the phenomenon occurs – are first pinpointed, and then implemented in the appropriate codes. For example, although failure of a component is usually considered as a macroscopic event, the main portion of damage incurred during irradiation occurs at a microscopic, or even nanoscopic, level. Determination of the local mechanical properties from the micro-structure is therefore of utmost importance, and indicates the need to approach the issue of using a multi-scale modelling scheme, which encompasses broad time and length scales. Scales begin at the atomic level, using, *ab initio*, molecular dynamics and kinetic Monte-Carlo techniques, and end at the larger spatial scales, where dislocation dynamics, FE methods, and, ultimately, more general continuum models are employed.

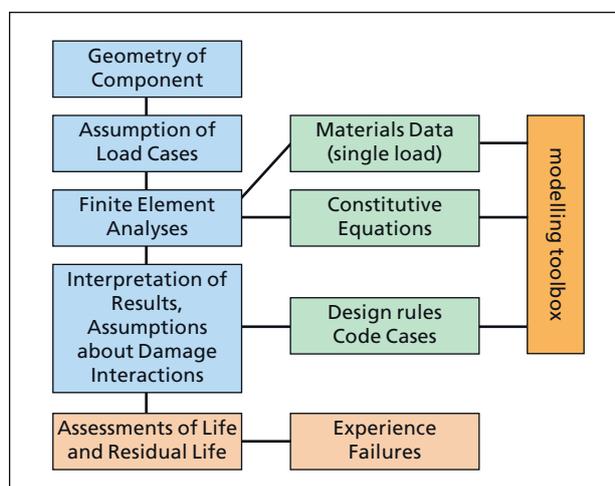


Figure 1: Schematic of the design process. [1]

As many of the phenomena take place on a time scale which cannot be reproduced in the laboratory, reliance has to be placed on modelling to enhance basic understanding, thereby improving the accuracy of design-life assessments. Modelling schemes starting from the smallest time and length scales and moving up through the scales to the macroscopic (i.e. a bottom-up approach) might appear to be a logical progression. However, we prefer to address material strength as the designer him/herself understands it (as a top-down process), looking first at the constitutive equations, going down a scale to the interaction of dislocations and their role in the mechanical behaviour of materials, and then moving to smaller scales. Such small scales are often not visible experimentally, and are frequently overlooked by designers. Nonetheless, their inclusion in materials research has become a reputable methodology for providing new insights into material behaviour.

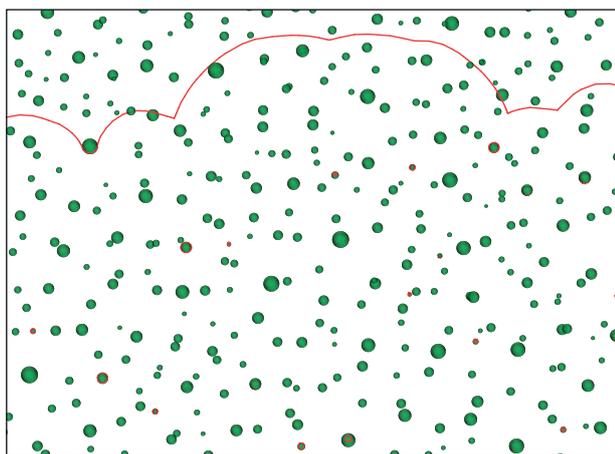


Figure 2: **Result of a DD simulation of a dislocation moving through the ferritic ODS alloy PM 2000.**

Oxide-dispersion-strengthened (ODS) steels are of prime interest for several high-temperature applications, as well as for advanced gas-cooled reactors, which are being investigated within the international Generation IV initiative [2]. For example, fine, ceramic (yttria) particles are dispersed in a ferritic matrix to provide obstacles for dislocation movement, thereby increasing material strength. Dislocation dynamics (DD) can be used to model such phenomena as shown in Figure 2, and the yield strength of the material thereby be determined. Optimal particle size and distribution can be studied, and the effects on material strength of additional phases formed during long-term operation, or from helium bubbles formed as a result of irradiation, can also be analysed. An extension of these studies to high temperatures and creep are necessary to understand material degradation in high-temperature reactors, particularly to mechanisms for dislocation obstacle interaction, dislocation/dislocation interaction, and diffusion-controlled dislocation movement. This requires modelling at

the atomic scale using the method of molecular dynamics (MD), together with kinetic Monte Carlo (kMC) techniques. MD and kMC methods can also be used to analyse point-defect movement, and other irradiation-induced material damage, which can become important during transient operations like reactor start-up. Questions of possible growth of creep-induced grain boundary voids by point defects created during irradiation can also be studied with MD/kMC. Proper MD simulations need physically correct inter-atomic potentials. The main elements of many high temperature steels and alloys are iron, chromium and nickel. The iron-chromium system is very important for high temperature steels, including the ODS alloy PM 2000. As iron and chromium have different magnetic properties, the question arises of the importance of using potentials containing a magnetic component. To study such issues, it is necessary to perform first-principle investigations; i.e. *ab initio* calculations. With proper potentials, technically very important information, such as phase diagrams, can also be modelled. Together with thermodynamics-based programs, good predictions of how phases can form with time are possible.

A multi-scale approach

From these considerations, it becomes obvious that reliable life-time models need to work over the full spectrum of dimensions; i.e. a multi-scale approach.

Of course, any modelling predictions must be experimentally validated; this also requires multi-scale information. Testing of miniature samples and advanced analysis techniques are necessary for this purpose, requiring a high resolution transmission microscope or beamline X-rays and neutrons. Although this concept looks rather straight-forward, much work is still necessary to develop a sound design tool for future use. Volumes capable of being modelled are small, and simulation times are short, even if supercomputing facilities are available. Consequently, the extension of the multi-scale approach to higher temperatures and longer times is a real challenge, necessitating international and interdisciplinary collaborations. The Center of Competence for Energy and Mobility (CEM-CH) provides a promising forum for such projects.

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Cation transport through compacted montmorillonite

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Despite decades of research, the mechanistic treatment of the diffusion of cationic species in swelling clays, used as a backfill material in the disposal of radioactive waste, is still a subject of controversy in the literature. Recent experiments at PSI indicate that at high degrees of compaction the diffusion of cations occurs predominantly through the interlayer porosity of the clay, and is driven by the concentration gradient of tracer cations in the interlayers. In contrast to conventional transport models, the chemical interaction of the cationic diffusant with the clay affects not only its retention behaviour, but also its mass flux.

Bentonites are being considered as the backfill material in which to embed canisters filled with long-lived intermediate-level radioactive waste, high-level waste, and spent fuel in tunnels of deep geological waste repositories. In addition to various mechanical functions, the role of the bentonite buffer is to retard, over long periods, the possible release of radionuclides into the far-field of the repository following canister failure. The clay fraction of bentonites is composed essentially of montmorillonite: a smectite-type clay mineral composed of layers of octahedrally coordinated aluminium, sandwiched between two layers of tetrahedrally coordinated silicon atoms in a 2:1 arrangement (often referred to as TOT sheets). An intrinsic property of these clays is their ability to swell in the presence of water, which leads to compacted bentonites with extremely low hydraulic conductivities. As a result of this compaction, migration of radionuclides is predominantly governed by the comparatively slow process of molecular diffusion.

The diffusion of charged species in compacted bentonites, compared with diffusion in free water, is largely influenced by its complex micro-structure and the high, fixed negative charges at the clay particle surfaces. Different physico-chemical states of water can be distinguished. Water may be present as ‘free water’ in the pore space between the clay platelets, and is then assumed to have similar properties to bulk water. In contrast, water present between the TOT sheets, the so-called *interlayer water*, is influenced by large numbers of positively charged cations compensating the negatively charged surface. For this reason, and because of the very small interlayer separation, the physico-chemical properties of interlayer water may be very different from those of the bulk water.

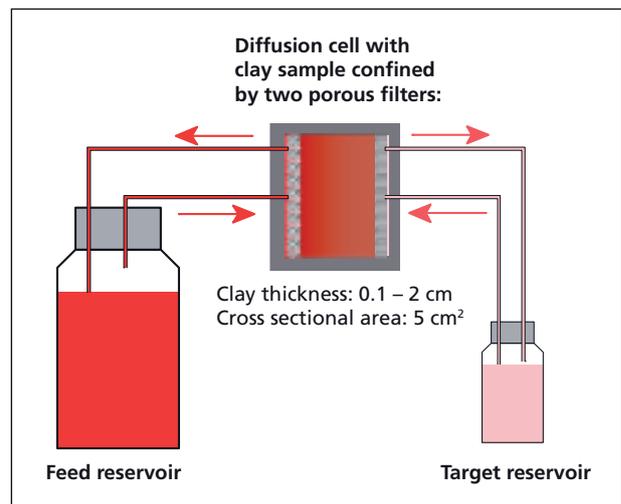


Figure 1: Schematic of a through-diffusion test.

Despite the fact that diffusion data are readily available for many radionuclides from the literature, detailed knowledge of the diffusion processes of charged species through compacted clays remains rather poor. The overall aim of the present work is to understand the driving forces behind the diffusion of cations in compacted montmorillonite. The special challenge is to establish empirical relations using indirect evidence, since the specific diffusion pathways cannot be tracked at the small scales involved, for lack of suitable instrumentation.

Experiments and interpretation

The diffusion of $^{22}\text{Na}^+$ and $^{85}\text{Sr}^{2+}$ was measured in highly compacted montmorillonite by the classical through-diffusion technique, combined with tracer profile analysis. A sche-

matic of the arrangement is given in Figure 1, and a photograph of the steel pressure cells used to confine the samples is shown in Figure 2. Nuclide transport through the clay sample from the feed to the target reservoir was measured as a function of time. The main result of these investigations was that the conditional diffusion coefficients (cD), calculated on the basis of the tracer concentration gradient in the aqueous phase in contact with the clay, and the sorption distribution ratios (R_d), were both found to decrease with increasing external salt concentration. In a logarithmic representation of these data, a slope of -1 was obtained for the monovalent ${}^{22}\text{Na}^+$, and a slope of -2 for the divalent ${}^{85}\text{Sr}^{2+}$, as indicated in Figure 3. Such an observation was somewhat unexpected. For the diffusion of sorbing species in porous media, two parameters are commonly used to model the mass flux: an effective diffusion coefficient and R_d . The maximum possible mass flux is a function of the effective diffusion coefficient and the concentration gradient of the species under consideration in the aqueous phase. The sorption distribution ratio only determines the time needed to reach the maximum possible flux. On such a basis, it is difficult to understand why the mass flux at steady-state should be a function of the external salt concentration. A possible explanation is that, for swelling clays at high degrees of compaction, the dominant pathway for cation diffusion is through the interlayer space. Further, the driving force determining the mass flux is the tracer concentration gradient in the interlayer itself [1]. This gradient is a function of the external salt concentration, since the tracer will distribute itself between the free pore water and the interlayer via cation exchange. This process is well known, and can be calculated. Effective diffusion coefficients based on such an interlayer tracer concentration gradient were found to be inde-



Figure 2: Diffusion pressure cells.

pendent of the composition of the external aqueous phase. This implies that in diffusion tests the interaction of cationic species with clay minerals affects not only the retention time but also the maximum possible mass flux. Future experiments are aimed at developing an integral treatment of the diffusion of anions and cations in clay minerals at different degrees of compaction.

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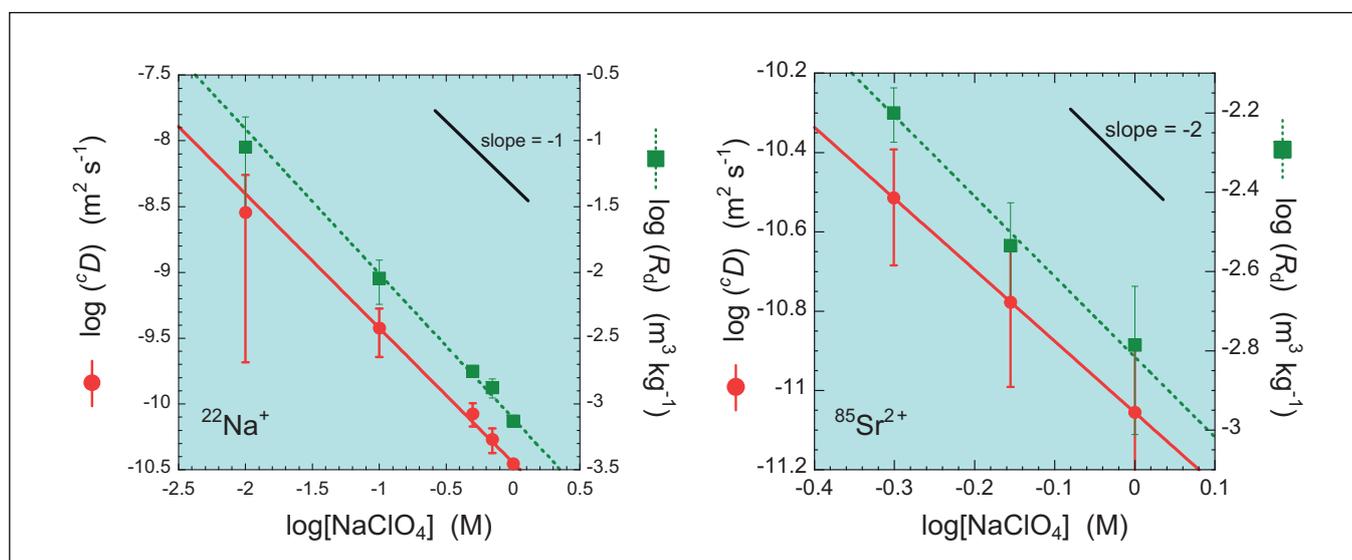


Figure 3: Logarithmic representation of the dependence of cD and R_d on the salt concentration in the water phase contacting the highly compacted montmorillonite for ${}^{22}\text{Na}^+$ and ${}^{85}\text{Sr}^{2+}$.

A probabilistic assessment of MEGAPIE safety

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A scoping-level probabilistic safety assessment (PSA) has been applied to selected systems of the Megawatt pilot target experiment (MEGAPIE) at PSI. In applying PSA to such a complex facility, a number of challenges arise, mainly related to the analysis of electronic and programmable equipment, and of one-of-a-kind components. Though the associated quantification shortcomings hinder a complete characterization of the risk profile, some level of importance/significance evaluation was feasible, such that practical and detailed recommendations on potential system improvements were derived.

MEGAPIE is an international experiment hosted at PSI to demonstrate the feasibility of a liquid lead-bismuth target for producing neutrons by spallation reactions [1]. Operation started on August 14, 2006.

A scenario of concern for the safety of MEGAPIE was an excessively focused beam, exposing the target window in the liquid metal container (LMC) to an excessive power density, which might eventually cause a breach of the container [2].

The work presented here builds on existing safety studies. Deterministic fluid dynamics and structural mechanics analyses had previously been carried out [3], providing the bases for the MEGAPIE safety concepts and requirements [2]. Possible sources of data for failure probabilities had also been investigated [4], and PSA used to evaluate relevant causes of LMC failure, together with the severity of different scenarios following the failure [5]. The latter study confirmed that target failure due to severe beam over-focusing was the most likely scenario to have serious safety consequences, thereby seriously jeopardizing the safe operation of the target.

PSA of experimental facilities: challenges

A first challenge comes from the extensive use of digital components and software systems, for which the prediction of failure modes is problematic, as experienced in aerospace and nuclear power plant applications [6].

In addition, experimental facilities often use one-of-a-kind components, designed specifically for the needs of the particular experiment. Past experience with similar components is also difficult to assess, because such components and the associated software are often revised to accommodate new hardware, fix errors, or add new functionality. The operating

environment and performance requirements may also differ. To address these issues, failure modes and effect analysis were used more extensively than is usual for more conventional applications. Further, given the quantification difficulties, emphasis was placed on the qualitative insights which could be obtained from the model, with the aim of evaluating the adequacy of the safety systems with respect to redundancy and diversity. The details of the PSA can be found in [7].

The PSA process

PSA is the implementation of a systematic search for those abnormal operational modes which could initiate accidents, or cause system failure. Accident sequence models are then compiled to represent the resulting scenarios.

Scenarios and initiating events of interest here are those that may lead to an excessively focused beam footprint. Three scenarios were considered: (1) bypass of the scattering Target E by the proton beam (designation TE-BY); (2) wrong settings loaded into the control devices of the quadruple magnets located underneath the MEGAPIE target (WSET1); and (3) failure of these quadruple magnets to set (WSET2). The accident sequence model for TE-BY is shown in Figure 1 as an example.

PSA results and discussion

The PSA results can be used to evaluate the adequacy of the safety systems with respect to redundancy and diversity, and thereby to gain safety insights and make recommendations on potential system improvements. The information was derived from the system minimal cutsets (MCSs), i.e. the minimal

combinations of failure events that, if they occurred, would lead to system failure, given that the corresponding initiating event had occurred. Inspection of the MCSs enables the existence of single, double, triple, etc. points of failure in the system to be identified. The main results of the PSA are listed here.

- The three monitoring systems [8] constitute a diverse protection mechanism against scenarios originating from bypass of Target E.
- The design of the system for processing the shutdown signals (the *Schnelles Abschaltssystem*, [9]) is redundant, and no independent single point of failure was identified.
- The VIMOS system [8], which visually monitors the light emitted by a glowing mesh heated by the beam, is involved in first-order cutsets associated with the WSET1 scenario, thus highlighting the importance of VIMOS as a protection against this scenario.

Recommendations derived from the results

Results from the PSA were used to make recommendations on potential system improvements. In particular, given the relevance of VIMOS to the safety of MEGAPIE, safety-related improvements were recommended to ensure that the VIMOS system was actively working.

Recommendation 1 (an administrative measure): formalize the daily routine checks in the control room to include a check of the status of the VIMOS system, to make sure it is functioning normally.

Recommendation 2 (a technical measure): implement an automatic check to additionally control that VIMOS is actively processing valid pictures. For example, a check can be performed whether the signal variance for different times is higher than a minimum value.

Conclusions

A difficulty in the application of PSA to experimental facilities concerns the analysis and quantification of the failure modes of electronic and one-of-a-kind components. As a result, emphasis was placed in this study on the qualitative insights that could be gained from the PSA. Quantification of probabilities of initiating and failure events to obtain a quantitative risk profile remains a goal for the future. An important step would be the collection and analysis of system and component test data, which, over time, would progressively reduce the uncertainties in the failure probabilities.

The work has demonstrated an approach for a scoping-level PSA that can be applied for experimental facilities. The results of this study for MEGAPIE have resulted in the implementation

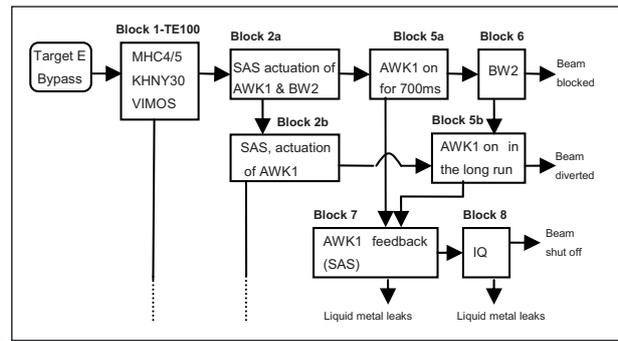


Figure 1: **Accident sequence model for total (100%) bypass of Target E (excerpt).**

of specific and practical measures oriented to enhance the safety of the facility.

Acknowledgements

The authors would like to thank Leonid Rivkin, Knud Thomsen, Timo Korhonen, Pierre Schmelzbach, Pierre-Andre Duperrex, Stefan Staudenmann and all the people of the MEGAPIE project for their support and helpful suggestions during the execution of this study.

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Climate-relevant cloud research in the Swiss Alps

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Anthropogenic aerosol particles partially counteract the warming effect of greenhouse gases by modifying cloud radiative properties. Elaborate in-cloud measurements of the partitioning of aerosol particles, cloud droplets and ice crystals were conducted in mixed-phase clouds at the high-alpine site Jungfraujoch. We found that the degree of glaciation strongly determines how many aerosol particles reside in the cloud droplets. Soot and dust particles were found to preferentially act as ice nuclei. These measurements are needed to improve the understanding of cloud formation and cloud persistence and to realistically initialize global models for a better prediction of climate change.

Interactions of aerosols with clouds

About 60% of the Earth's surface is covered with clouds at any one time. Clouds are an important regulator of the Earth's global temperature, because they reflect shortwave radiation from the sun back to space (cooling effect) and absorb long-wave terrestrial radiation from the Earth surface (warming effect). In the atmosphere cloud droplets can only be formed on suspended aerosol particles which provide a surface for the water vapour to condense on (Figure 1). The subset of aerosol particles that lead to the formation of cloud droplets

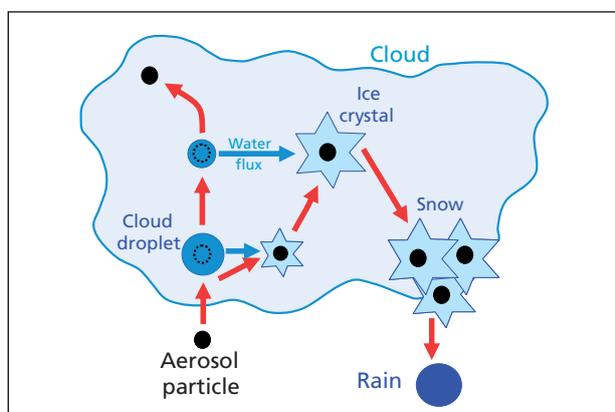


Figure 1: **Partitioning of aerosol particles, droplets and ice crystals in mixed-phase clouds. The ice crystals grow to larger sizes, because the water vapour preferentially condenses on ice rather than on liquid water (Wegener-Bergeron-Findeisen process). As a consequence the droplets evaporate and release aerosol particles back into the interstitial phase.**

are called cloud condensation nuclei (CCN). In our latitudes, most tropospheric clouds are mixed-phase clouds in which ice crystals and supercooled, liquid droplets coexist. Ice crystal formation is induced by particular atmospheric aerosol particles, called ice nuclei (IN), which provide the required surface for the initiation of the freezing process. An important pathway is freezing of existing supercooled droplets by contact with an IN. In recent years, the formation of ice crystals inside such clouds has moved into the focus of atmospheric cloud research, as the formation of ice inside clouds efficiently initiates precipitation (and thus shortens cloud lifetime) and influences the internal structure of clouds, which affects their cooling and warming capabilities.

Field measurements at the Jungfraujoch

The High Alpine Research Station, Jungfraujoch, offers an excellent opportunity to study liquid and mixed-phase clouds since it is located at 3500 m altitude, and is situated in clouds about 40 percent of the time. In international collaborations, a series of intensive field experiments were carried out from 2001 to 2007 at the Jungfraujoch station under the name CLACE (Cloud and Aerosol Characterization Experiment). For several weeks in a row a large set of instruments was deployed in order to investigate the microphysical parameters (concentration and size) and chemical composition of cloud drops, ice particles and aerosol particles (Figure 2).



Figure 2: Measurement of aerosol size distributions.

Characterization of ice nuclei (IN)

In order to investigate aerosol particles that served as IN, small ice crystals were continuously sampled inside clouds and separated from supercooled droplets and from the interstitial aerosol particles, i.e., those that did not form droplets or ice particles. This extraction was achieved with an Ice-Counterflow Virtual Impactor (Ice-CVI), which was developed at the Leibniz-Institute for Tropospheric Research, Germany. Downstream of this instrument, the IN on which the ice crystals formed were analyzed with sophisticated instrumentation. The number concentration of IN as well as their size and chemical composition was compared to the same parameters derived from analyses of supercooled drops, interstitial and total aerosol particles sampled by other inlets.

It was confirmed that only a very small subset of atmospheric particles serve as IN (approximately 1 IN per cm^3 of air,

while a typical total aerosol particle concentration is 1000 particles per cm^3). With respect to the total aerosol particles, the larger ones ($> 300 \text{ nm}$; $1 \text{ nm} = 10^{-9} \text{ m}$) preferentially act as IN. In contrast to this, particles that form cloud drops, CCN, are found at sizes as low as 60 nm and are present at much higher concentration (approximately 100 CCN per cm^3).

From the chemical analysis (Figure 3) it becomes obvious that the chemical composition of ice nuclei is remarkably different from the total aerosol (i.e. the background aerosol that is present before a cloud forms). The total aerosol consists mainly of water-soluble substances like sulphate, nitrate, ammonium and various organic substances, whereas insoluble and refractory materials like mineral dust and soot (black carbon) are identified as IN. All these substances (except mineral dust) are mainly produced by human activities. The finding that these particles favour ice formation is of particular importance for climate modelling.

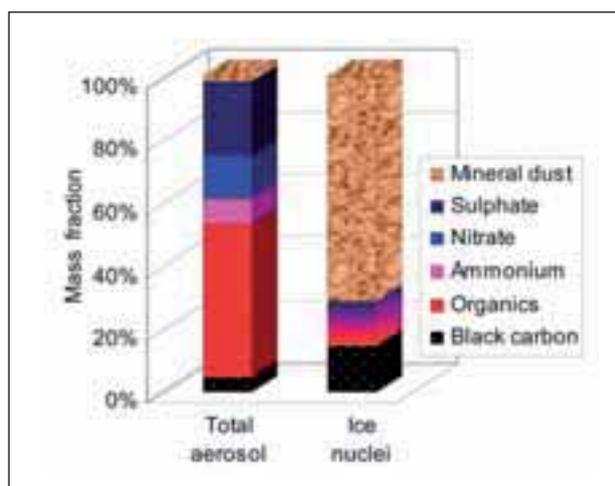


Figure 3: Chemical composition of sub-micrometer-sized aerosol particles. Total aerosol is the whole aerosol particle population that is available for cloud formation. Ice nuclei are the subset of the total aerosol which initiate the formation of ice crystals in a cloud. Mineral dust and soot particles (black carbon) are more abundant in ice nuclei indicating that these particles play a central role in initiating ice formation.

Global modelling and future activities

The observed relation among the number concentration of ice crystals, the particle number concentration and the ice mass fraction are currently implemented into a global climate model at ETHZ for a better prediction of future climate. First model runs suggest that the observed partitioning results in a stronger net indirect effect of aerosols on climate.

The observation that soot particles preferentially act as IN implies a direct anthropogenic impact on ice formation in clouds. The consequences for the initiation of precipitation and for global warming are not yet clear, but the results show that an accurate radiative energy balance requires correct treatment of the ice phase in the models.

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Sunlight and gases compete within the tiny world of aerosol particles and ice surfaces

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Interactions of trace gases with liquid and solid material in aerosol particles, cloud droplets or on the ground are relevant to our climate, the ozone budget and human health. In this report, we show that the chemistry in the complex microenvironment is characterized by competition between gas and condensed phase reactants. This competition, as shown here for organic aerosol particles and for ice of relevance to arctic snow packs, may affect atmospheric chemistry and climate.

Introduction

Solid and liquid material are dispersed in many different forms in the atmosphere and on the ground, while at the same time being exposed to a large variety of major and trace gases in the air. The chemical interactions of trace gases with these materials are relevant to the climate, the ozone budget and human health. A thorough understanding of such effects on local, regional and global scales requires knowledge about the fundamental chemical processes involved on a molecular level.

Ozonolysis of unsaturated fatty acids

Unsaturated fatty acids are abundant constituents of biomass and its degradation products. They have been detected in both natural and anthropogenic aerosol particles, for example components of oil in emissions from cooking activities. Oxidation of these compounds in the atmosphere occurs through ozone attacking the double bonds characteristic of these compounds. The first stable products in this complex degradation mechanism, the Criegee intermediates (CI), react further to produce multifunctional carboxylic acids, aldehydes, large molecular weight peroxides and polymers. The smaller acids among these products are soluble and contribute to the hygroscopicity and the ability of the particles to act as cloud condensation nuclei.

In fact, using particles consisting of arachidonic acid, a C_{20} compound with four double bonds as a proxy of fatty acids, we have observed that the hydrophobic particles are getting

hygroscopic when exposed to atmospheric levels of ozone. Hygroscopicity is quantified in terms of the hygroscopic growth factor, which is the diameter of the particles measured at a given humidity divided by its diameter under dry conditions. It can be related to the presence of solutes in the particles. In more detail, we have demonstrated that exposure of arachidonic acid particles to ozone under humid conditions leads to more hygroscopic growth than under dry conditions (see Figure 1). At the same time, the concentration of carboxylic acids in the oxidized particles strongly correlated with the hygroscopic growth. This ratio has been measured using proton nuclear magnetic resonance (1H -NMR) of particle samples. We suspect that in the initial stages of the degradation mechanism, water successfully competes with other

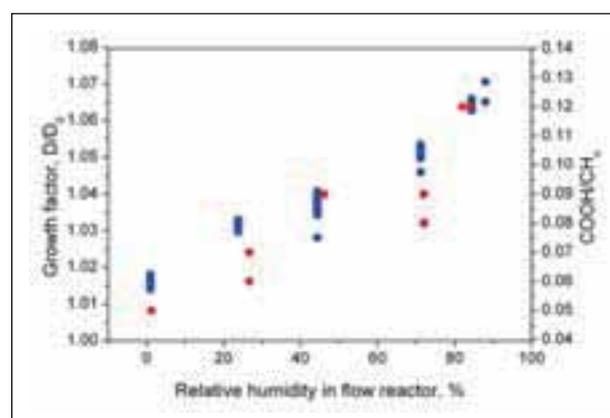


Figure 1: **Hygroscopic growth factor at 90% humidity (●) and ratio of carboxylic to aliphatic carbon (●) of oxidized arachidonic acid particles as a function of the relative humidity during exposure to ozone.**

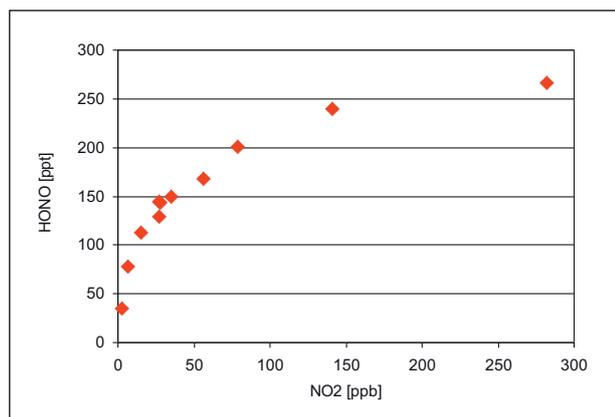


Figure 2: **Formation of HONO from the reaction of NO₂ with submicron humic acid aerosol particles in presence of visible light as a function of the NO₂ concentration in the flow reactor, demonstrating the competition among electron acceptors.**

acids and intermediates for reaction with the Cl, leading to more of the smaller acids. This has important implications for the condensed phase alkene chemistry in organic aerosol particles and their effects on climate.

Photosensitized reduction of NO₂

We have recently discovered a new pathway of heterogeneous production of nitrous acid (HONO), where nitrogen dioxide (NO₂) is reduced to HONO by photoactivated organic films, such as humic acids, or soil [2]. HONO is an important precursor of OH radicals, the major oxidation agent in the atmosphere. The proposed mechanism includes absorption of light by an aromatic ketone, oxidation of reduced aromatic moieties and transfer of an electron and a proton to NO₂. We have now been able to follow this photosensitized reaction on submicron humic acid aerosol in an irradiated flow reactor mimicking daylight conditions. We observed a non-linear increase of the HONO formation rate with increasing NO₂ concentration. We attribute this saturation behaviour to competing electron acceptors associated with the aerosol that lead to deactivation of the electron donors and thereby limit the reaction rate with NO₂.

Co-adsorption of acids on ice

Snow and ice are very important surfaces in our environment. During part of the year, more than 50% of the landmass of the northern hemisphere is covered by snow or ice. It has recently been recognized that this ice is an important substrate acting as a source and sink for trace gases and therefore significantly affects atmospheric chemistry [3]. We have re-

cently investigated partitioning of nitrous acid (HONO) to ice. In these experiments, we observe the migration of HONO molecules labelled with the short-lived radioactive isotope ¹³N along a packed ice bed as a proxy of snow. Chromatographic retention driven by adsorption and desorption leads to progressive decay along the ice surface (see Figure 3). The slope is directly related to the coverage and the adsorption properties. In the present experiments, we compared such profiles of labelled HONO molecules in presence and absence of acetic acid. Acetic acid is an abundant product from the photochemical degradation of organic compounds. As shown in Figure 3, the presence of this acid significantly lowers and flattens the profile of HONO. The two acidic species clearly compete for available adsorption sites, and we also suspect that their conjugated bases compete for protons on the ice surface, where the availability of free water molecules is limited.

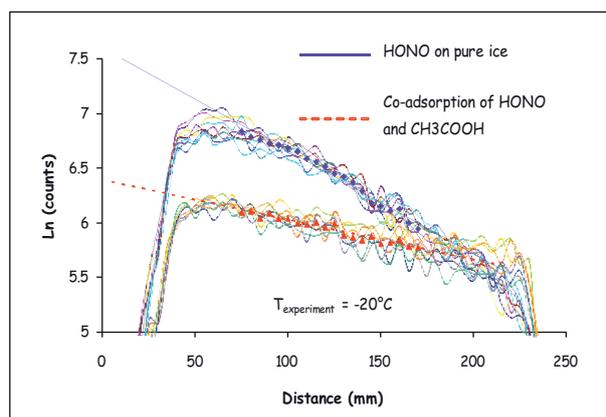


Figure 3: **Profiles of HONO labelled with the short-lived isotope ¹³N (with a half-life of 10 min.) along a packed ice bed in presence and absence of acetic acid. The profiles are scanned repetitively every 3 min. Only profiles after a steady state has established are shown (typically after 30 min).**

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Beaming in on radioactive materials: microXAS

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Synchrotron-based X-ray absorption spectroscopy (XAS), X-ray fluorescence (XRF) and X-ray diffraction (XRD) have become key analytical techniques in many fields of basic and applied science, and now have a major impact on the exploration of chemical reactivity and structural identity of both engineered and natural systems. As a result of improvements in X-ray sources, X-ray optics, detector technology and sample positioning, XRD, XRF and XAS now give access to a wealth of structural and chemical information at the micrometer scale, opening up the potential to probe not only small and heterogeneous, but also dilute samples. This suite of powerful analytical tools has recently become accessible to the nuclear science community. The development and application of a modular shielding concept, in combination with the temporary establishment of a controlled radioactive zone, has enabled X-ray microprobe analysis of radioactive samples to become available at the microXAS beamline.

The unique potential of X-rays for the characterization of materials was recognized almost immediately after their discovery in 1895 by W.C. Röntgen. The manner in which X-rays interact with matter permits, for example, complex molecular structures to be examined by means of scattering or diffraction experiments, thereby enabling atomic-scale resolution to be achieved. Without doubt, the capability to determine element-specific chemical properties, such as local coordination environments and oxidation states, by means of X-ray absorption spectroscopy is also of fundamental importance.

With the increasing recognition that macroscopic material properties and chemical reactivity may be traced back to nano- and micro-scopic processes, the need for X-ray microscopes has grown rapidly. However, the successful micro-focussing of X-rays remains a considerable optical and technical challenge.

New technology allows breakthrough

The realization of efficient X-ray microprobes had to wait until the availability of the most modern light sources. These so-called *Third Generation Synchrotrons*, such as the Swiss Light Source (SLS), are characterized by small source sizes, high photon fluxes, and low beam divergences. At the same time as the realization of these high performance light sources, remarkable breakthroughs were achieved in X-ray optics. The

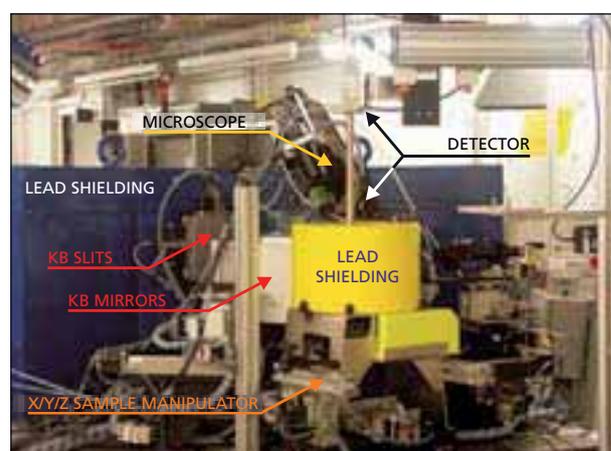


Figure 1: **Experimental set-up for the measurement of active samples at the microXAS beamline.**

simultaneous advancement in these two areas has resulted in a significant increase in the available photon flux and flux density within X-ray microprobes.

Based on the initiative and under the direction of the Laboratory for Waste Management (LES) at PSI, a high-resolution, hard X-ray microprobe station has been built at SLS: namely, the *microXAS beamline*. This analytical facility enables investigation of materials and matter to be carried out with a spatial resolution of approximately $1\mu\text{m}^2$. Most important is

the capability of the instrument to determine chemical speciation within single micro-domains, in addition to the local structural analysis.

The uniqueness of the microXAS beamline is that it enables radioactive materials to be investigated – a capability that hardly any X-ray microprobe facility around the world can rival.

X-ray microprobe analysis of radioactive samples

The first experiments involving radioactive samples have recently been conducted. In collaboration with PSI-internal and international partners (e.g. PSI-LWV, CEA [F], ITU [D], STUDEVIK[S]), a variety of active samples have been examined using a micro-focused X-ray beam. The beam was focussed using Kirkpatrick-Baez (KB) mirrors to a spot size as small as $3 \times 3 \mu\text{m}^2$. For most samples under investigation, elemental distribution maps were recorded by collecting two-dimensional micro-XRF data, and the first series of microXAS spectra of radioactive specimens was also collected.

The different experimental campaigns were undertaken in compliance with the microXAS radioactive safety procedure, as approved by the Federal Office of Health (*Bundesamt für Gesundheit, BAG*). A 'Type 1' radio-active zone was set up at the microXAS beamline. This included environmental monitoring, a controlled gas exhaust system, a sample holder, hand-and-foot monitor, and additional local shielding. After completion of the experiments, mandatory non-contamination checks were performed in the experimental hutch, after which the zone was temporarily removed.

An impression of the complex experimental set-up can be obtained from Figure 1. Most noticeable is the removable local shielding (coloured blue and yellow), which was installed during the investigation of active specimens to provide protection against γ -emissions.

First results

An illustrative example of X-ray microprobe investigation of a radioactive specimen is depicted in Figure 2. A heterogeneous cement sample containing several heavy metals, including ^{60}Co , was solidified in a cement matrix (total activity 1300 Bq, with dose rate $2 \mu\text{Sv/h}$ at 1 cm). After hardening (hydration) of the cementitious waste slurry, the spatial distribution of different chemical elements was determined by means of micro-XRF. The left panels of Figure 2 show the distribution patterns of nickel and iron obtained. The Figure nicely demonstrates the microscale heterogeneity within the cement matrix, and reveals also the heterogeneous distribution pattern of nickel (and other chemical elements) after solidification. The immobilisation of Ni in a cement matrix results in Ni-rich micro-domains ('hot spots').

Micro-EXAFS experiments were conducted on a Ni-rich spot, localized within the cement matrix by antecedent microXRF mapping. Such micro-spectroscopic investigations enable the chemical speciation of nickel in the heterogeneous cement matrix to be determined. Figure 2c shows the k^3 -weighted Ni K-edge EXAFS spectrum. The chemical speciation observed in the radioactive cement specimen is compared with bulk measurements of Ni reference compounds: namely, $\alpha\text{-Ni(OH)}_2$, a natural takovite sample, and a synthesized Ni- Al_2 -layered, double hydroxide (LDH). Although a more comprehensive data analysis is still ongoing, preliminary conclusions can already be drawn, the most important being that during the hydration process a major part of the aqueous Ni is immobilized in the form of a secondary, highly insoluble, Ni-Al LDH precipitate.

Detailed knowledge concerning the structural micro-heterogeneity and chemical speciation is of central importance for assessing the long-term behaviour and stability of the waste matrix: for example, in the context of the safety assessment of nuclear waste deposits.

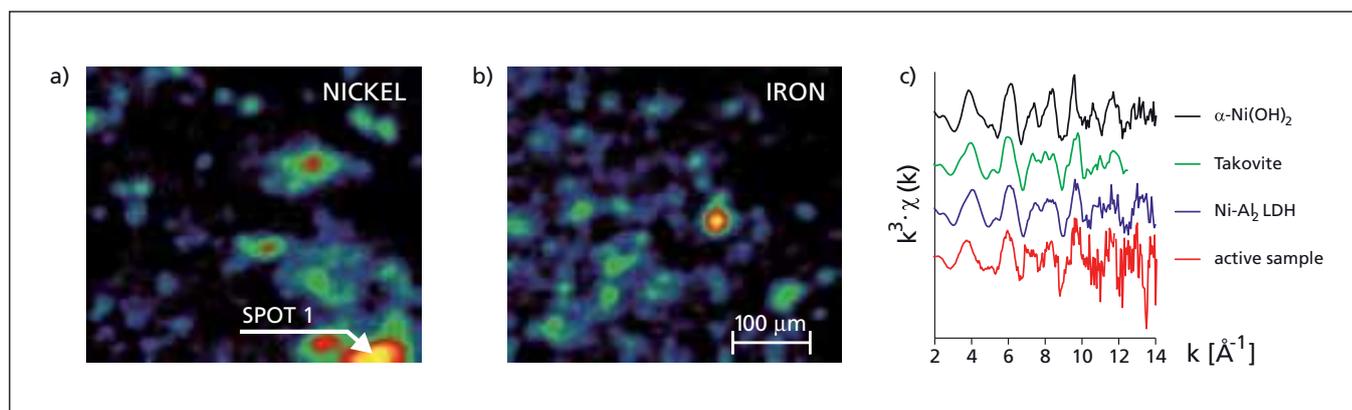


Figure 2: Micro-XRF results showing the spatial distribution of (a) nickel and (b) iron within a radioactive Ni-doped cement sample, together with the spectroscopic data (c).

Swiss electricity supply options in focus

Stefan Hirschberg, Christian Bauer, Peter Burgherr, Roberto Dones, Thomas Heck, Warren Schenler,
Laboratory for Energy Systems Analysis, PSI

The sustainability of the current and future power-supply technologies relevant to Switzerland has been analyzed within the context of a comprehensive, interdisciplinary study. The evaluation is based on both the total-cost approach, and on the multi-criteria aggregation of ecological, economic and social indicators. The use of total costs leads to a clear ranking of the technological options, with the social dimension represented only to a limited extent. In contrast, the ranking resulting from the multi-criteria approach explicitly incorporates a wider spectrum of social aspects as well as stakeholder preferences.

The goal of the study was to produce an interdisciplinary evaluation of current and future electricity-generating systems, operating under Swiss-specific conditions. The project was coordinated by the major Swiss energy supplier, Axpo. In addition to PSI, the participants included the University of Stuttgart, the Centre for Energy Policy and Economics (CEPE) at the Swiss Federal Institute of Technology, Zurich (ETHZ), and BAK Basel Economics.

Scope and methods

The sustainability assessment employing Multi-Criteria Decision Analysis (MCDA) was defined in terms of a total of 75 criteria, with the associated indicators quantified for the years 2000 and 2030. To a large extent, current technologies were taken from the best commercially available options, while a wide spectrum of evolutionary concepts was included for the future technologies. Compared to earlier studies, which focused on power technology assessments in Switzerland [1], Germany [2] and China [3], the present work embodies much greater diversity of technologies, and employs a much broader set of evaluation criteria and indicators.

Along with the modelling of power plants and their associated energy chains, the task of PSI included the full ecological aspect, as well as numerous social and economic criteria. The principal ecological criteria are greenhouse-gas emissions, consumption of resources, waste, and impact on ecosystems. PSI's contributions to the economic and social indicators consisted, among other elements, of providing estimates of electricity generation costs, as well as damage to health resulting from both normal plant operation and severe accidents.

Life Cycle Assessment (LCA) forms the basis for the quantification of ecological indicators. The approach does not take into account site dependencies, though this aspect is covered within the quantification of health and environmental damage due to air pollution from the various energy chains, which is based on the state-of-the-art *Impact Pathway Approach*, as defined in recent projects within the ExternE-series [4,5]. The background LCA database was ecoinvent v1.2, reflecting conditions in year 2000 [6].

The analysis of accident risk is based on historical experience (as reflected in the PSI database ENSAD [7]), and site-specific, simplified Probabilistic Safety Assessment (PSA). Economic indicators are built on extensive literature studies, earlier experience, input from industry, and, where appropriate, on expert judgement.

Selected results

Results presented here are based exclusively on the work at PSI. Figure 1 shows environmental indicators for the year 2030. For each indicator, the results are normalized (with 100% assigned to the worst-performing technology). Hydropower is superior in terms of minimal environmental impact; otherwise, the picture is diverse.

The total cost of electricity supply (internal production costs plus external costs resulting from health and environmental damage) constitutes a possible aggregate measure of sustainability (Figure 2). Nuclear power has the lowest total costs, both now and in 2030. External costs of fossil-fuel technologies are dominated by the damage caused by global warming (though estimates of this are highly uncertain). Some of the

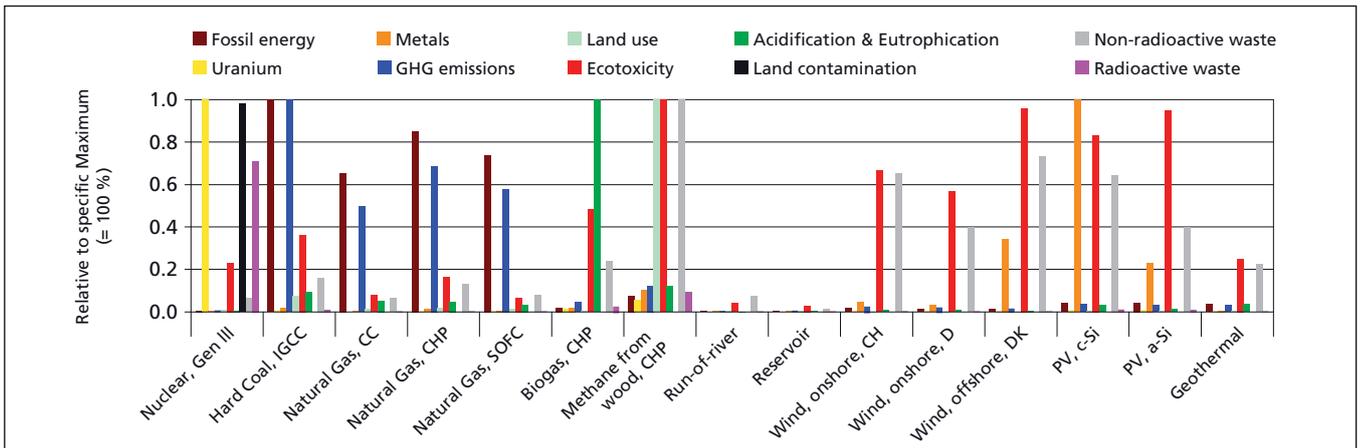


Figure 1: Environmental indicators for electricity generation in 2030 (not all of the options analysed are shown). Gen III = 3rd generation reactor; IGCC = Integrated Gasification Combined Cycle; CC = Combined Cycle; SOFC = Solid Oxide Fuel Cell; CHP = Combined Heat and Power.

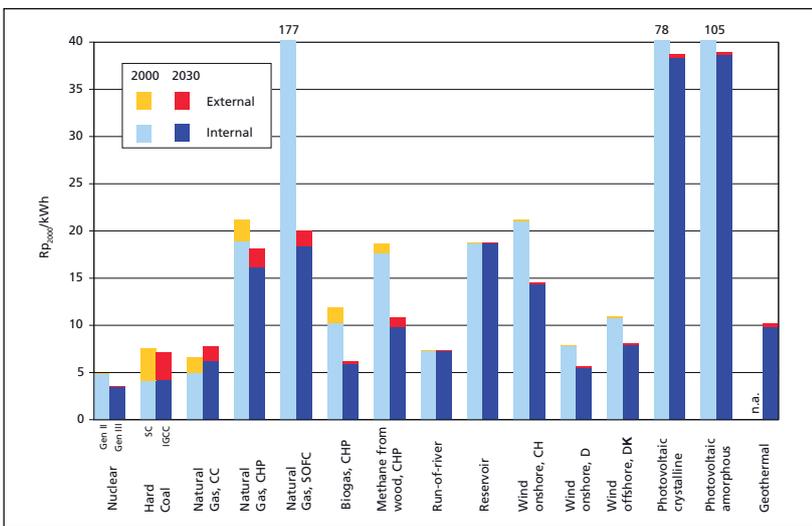


Figure 2: Full costs of electricity generation options in 2000 and 2030. (Gen II/III = Generation II and III reactors; SC = Supercritical; IGCC = Integrated Gasification Combined Cycle; CC = Combined Cycle; CHP = Combined Heat and Power; SOFC = Solid Oxide Fuel Cell)

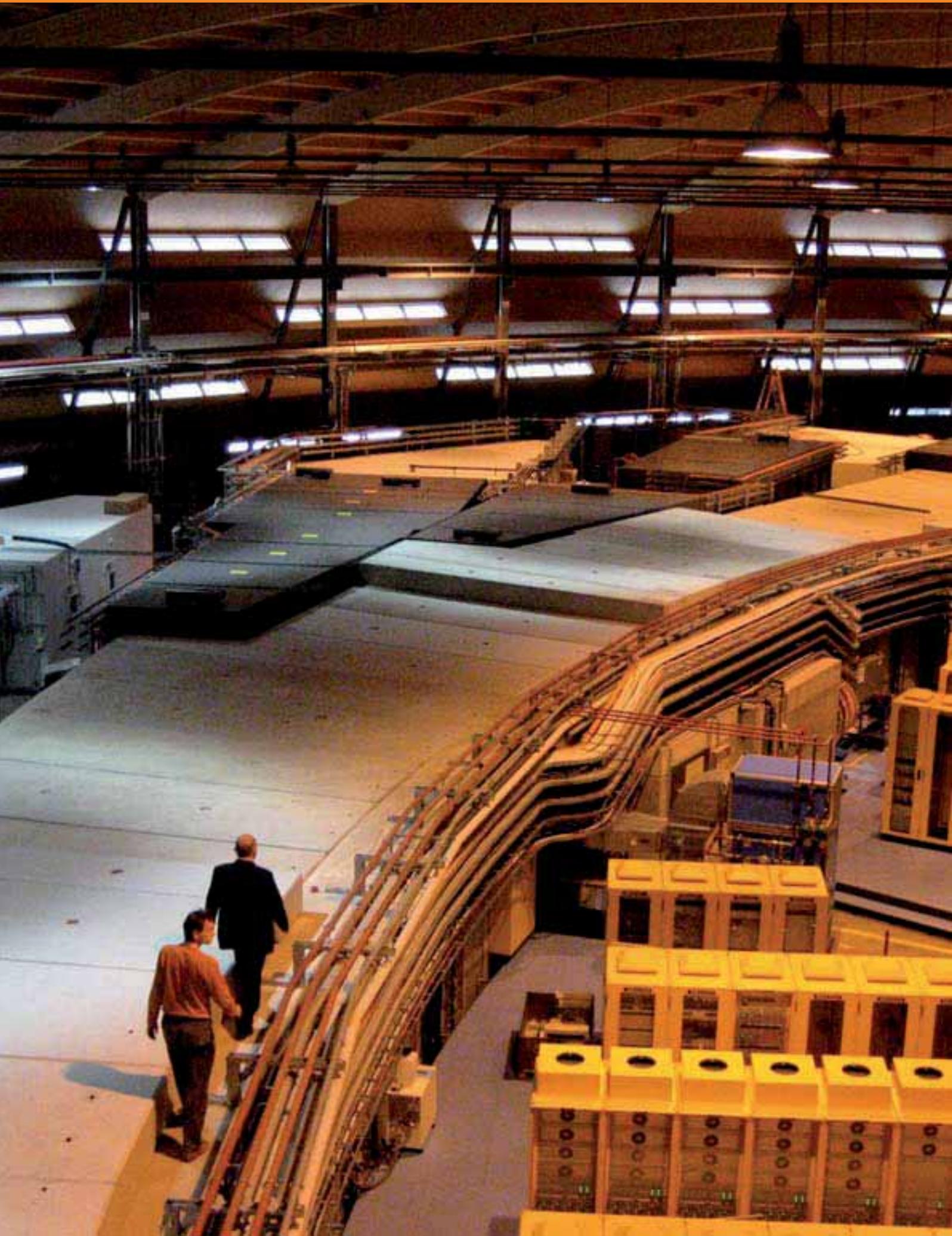
currently expensive renewable options will become more competitive later. Consideration of external costs improves the competitiveness of the renewables and nuclear power options in comparison to those based on fossil fuels.

The total cost approach is very useful for carrying out cost-benefit analyses, but its use in the assessment of the relative sustainability of the various options is not yet fully accepted. The main objections derive not only from limited coverage of social aspects, but from the acceptability of monetary values being applied to a few of the social indicators that have been explicitly addressed. Consequently, MCDA has been employed to provide an alternative quantification of the aggregate sustainability indicator. The complete MCDA model, with 75 criteria (some not readily amenable to monetization: e.g. risk perception and political stability), does allow for the consideration of individual or group preferences through assignment of appropriate weighting factors.

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User facilities 101

- 102 Swiss Light Source SLS
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- 108 Swiss Muon Source μS
- 109 Tandem accelerator
- 110 Proton accelerator
- 114 PSI-XFEL

Fully booked as usual

PSI provides unique research facilities to teams working on structural and condensed matter research. On one site we offer three essential tools, muon spin resonance (μS), neutron beams at SINQ and high brilliance photon beams from the SLS. Over 2000 external and in-house researchers, aided in their work by the PSI scientific and technical staff, and by the User Office, benefited from the state-of-the-art particle and photon beams.

The Swiss Light Source at PSI offers not only extremely stable beams of continuously tuneable X-rays, but also very short (on the order of 100 fs) pulses of hard X-rays. The world's highest power proton beam is used to provide very high flux neutron and muon beams. The experimental facilities for nuclear and particle physics with high-flux meson beams and the pilot project PROSCAN for clinical application of innovative cancer therapy with protons further enhance the reputation of PSI for scientific excellence (p. 110). PSI is heading towards a new generation of accelerators for research: the X-ray free electron laser (PSI-XFEL see p. 114).

Highlights achieved in 2006, as well as delivered performance records of the experimental facilities and of the accelerator systems providing the particle and photon beams, are reported in these pages. A wealth of important knowledge on high-flux spallation neutron sources for research and for nuclear transmutation will arise from the world's first megawatt liquid metal target experiment MEGAPIE performed in 2006 at PSI.

The SLS is one of the largest research facilities at PSI and much in demand by research teams the world over.

(Photo: Beat Gerber)

Operation of the Swiss Light Source in 2006

Andreas Lüdeke, *Department of Large Research Facility, PSI*

The Swiss Light Source has been enhanced in 2006 in terms of diagnostics, feedbacks and time resolution of experiments. A low coupling of about 1‰ has been reached and therefore a vertical emittance of about six picometre radian. A few long outages led to a slightly reduced availability and beam integral. Two major outages caused more than half of the downtime.

Operation and development

The year 2006 presented many highlights. One major milestone was the successful commissioning of the Femto beamline. The desired time resolution of better than 200 fs has been verified and first experimental results using these ultra-short X-ray pulses have been published. [1][2]

First operation started for the X-ray tomography beamline TOMCAT and for the soft X-ray beamline POLLUX, focusing on studies in polymer physics. POLLUX will use fast switching local vertical orbit bumps for experiments with synchrotron light of alternating polarization. Skew quadrupoles will provide a local coupling correction for those orbit bumps.

A special diagnostic beamline has been built to provide a precise beam size measurement in real-time. It allows resolving the extremely small height of the beam with a resolution of better than 1 μm at the source point. Due to this high resolution it was possible to optimize the beam coupling down to about 1‰ and to reach a vertical emittance as low

as 6 picometre radian for standard user operation. This now provides a tool that is more sensitive to transverse changes of the synchrotron radiation source than any of our user beamlines.

The multi-bunch feedback has been commissioned and is now another very important enhancement of the storage ring. The longitudinal feedback enabled us to suppress instabilities driven by higher order modes of the RF cavities. The transverse feedbacks are used to further reduce the small residual closed orbit distortions due to the top-up mode, thus becoming negligible for most experiments.

The average availability of the SLS synchrotron beam was 95%. The downtime was dominated by two major failures.

A broken RF ceramic window caused 37 hours of downtime after the April shutdown. Another 27 hours were required after the downtime to allow for the thorough startup of the beamlines. A broken 16 kV transformer of the site power caused another 67 hours of downtime at the end of October, just before a shutdown.

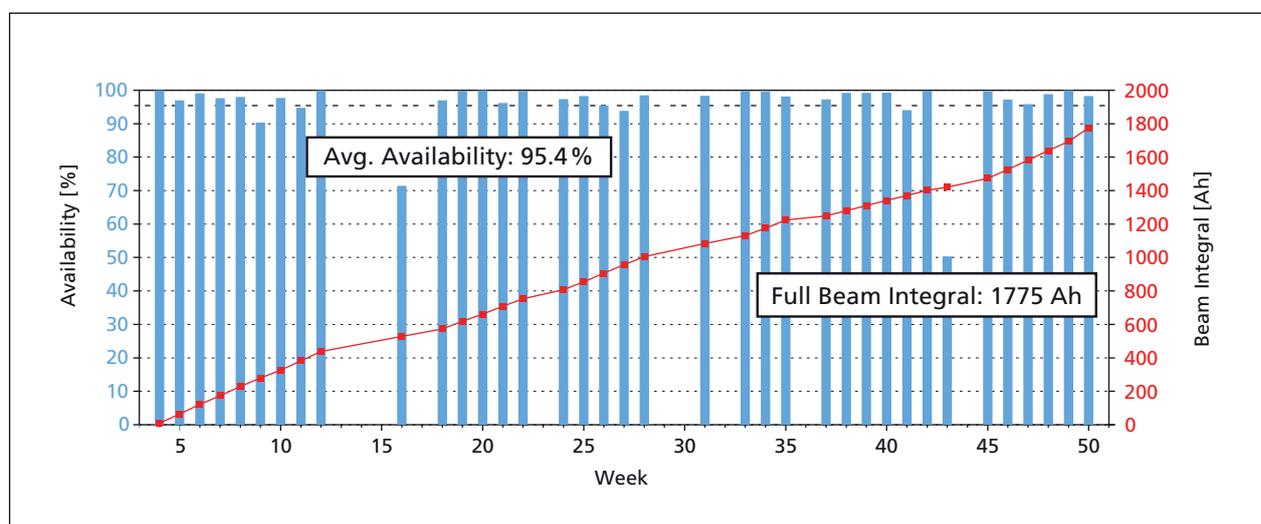


Figure 1: SLS operation statistics: weekly availability and integrated beam dose.

The integrated beam dose was 20% lower than the year before due to various problems with the RF system. The beam current was limited to less than 200 mA for 7 weeks due to a failure of a helium turbine of the cryostat system of the 3rd harmonic cavity. Higher order modes of the cavities and other RF problems forced us to run half of the year at about 300 mA instead of the standard 350 mA mode. The same problems prevented us to start operation at the design beam current of 400 mA.

Operation Statistics

The operational data is summarized in Table 1. Although the total downtime increased by nearly a factor of three compared to 2005, the mean time between failure was still at a good 60 hours. Figure 2 shows the reason for this: the total downtime was dominated by very few events. Without the five events longer than five hours, the total downtime would have been the same as in 2005. Again the majority of the downtimes have been below 30 minutes. The injector outage decreased again to now 26 hours. The outages were clearly dominated by Linac RF failures which added up to 60% of the total injector failure time.

The assignment of the downtime to the different systems is shown in Figure 3. Again the RF has been the reason for most downtimes in 2006. But in total the outages of the mains supply caused more downtime than the RF: one 16 kV transformer short circuit and four transient power cuts caused in total 82 hours of downtime.

Outlook

The year 2007 will be a busy year at the SLS. The new beamlines IR, VUV, ADDRESS, cSAXS, SuperXAS and PX-III will start operation. The tomography beamline TOMCAT changes from a normal bending magnet to a 2.9 Tesla ‘superbend’, providing a critical energy of 11 keV. And the Lucia beamline will be moved to the SOLEIL accelerator in France at the end of the year, giving space for Lucia II.

References

- [1] G. Ingold et al., “Sub-Picosecond Tunable Hard X-Ray Undulator Source for Laser/X-Ray Pump-Probe Experiments”, Proceedings SRI 2006, Daegu, Korea.
- [2] A. Streun et al., “Sub-Picosecond X-Ray Source FEMTO at SLS”, Proceedings EPAC 2006, Edinburgh, United Kingdom.

Beam Time Statistics	2006		2005	
<i>Total beam time</i>	6768 h	77.3 %	6608 h	75 %
• user operation	5160 h	58.9 %	4952 h	56 %
– incl. compensation time	144 h	1.7 %	175 h	2 %
• beamline commissioning	696 h	8.0 %	792 h	9 %
• setup + beam development	804 h	10.3 %	864 h	10 %
<i>Shutdown</i>	2168 h	22.7 %	2152 h	25 %
<i>User operation downtimes</i>	84		67	
• unscheduled outage duration	236 h	4.8 %	82 h	1.6 %
• injector outage (non top-up)	26 h	0.5 %	30 h	0.6 %
<i>Total beam integral</i>	1775 Ah		2129 Ah	
<i>Availability</i>	95.4 %		98.4 %	
<i>Availability after Compensation</i>	98.2 %		101.6 %	
<i>MTBF (mean time between fail.)</i>	60.0 h		73.0 h	
<i>MTTR (mean time to recover)</i>	2.8 h		1.2 h	

Table 1: **SLS Operation Statistics: two beam interruptions that occur within one hour are counted as one long downtime, because those short uptimes are generally not useful for experiments. This is relevant to the downtime and the mean time to recover (MTTR). However for the statistics in Figures 2 and 3 each beam interruption is counted individually.**

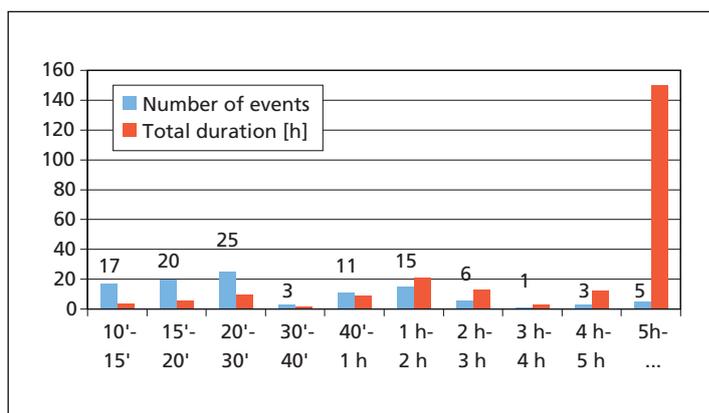


Figure 2: **Downtime events per time to recover.**

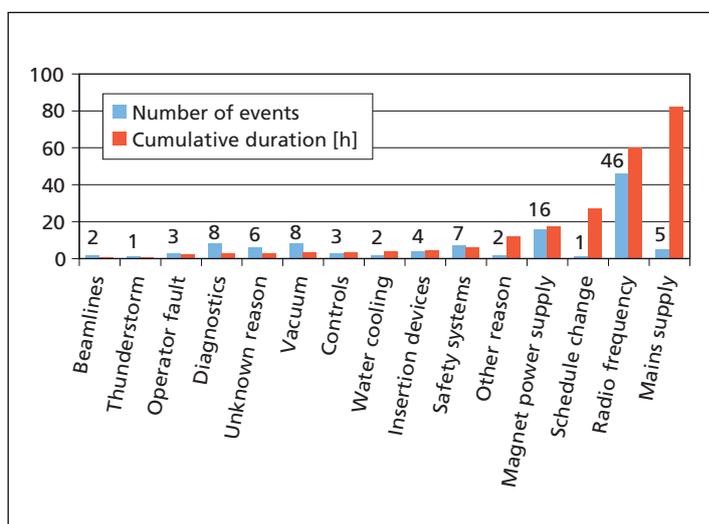


Figure 3: **Downtime events and duration per system.**

SINQ: the continuation of a success story

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The year 2006 was very exciting for the operators and users of the Swiss Spallation Neutron Source (SINQ). The worldwide first 1 MW liquid metal spallation target (MEGAPIE) was installed and thereafter successfully and reliably operated for more than four months. The SINQ users greatly benefited from the neutron flux gain of 80% at the instruments and performed 260 experiments in the relatively short operational period. Another milestone was reached by detecting the first neutrons at the new backscattering spectrometer MARS, which will be available for user experiments in 2007.

MEGAPIE: a neutronic pilot experiment

SINQ, the Swiss spallation neutron source, is driven by PSI's 590 MeV proton accelerator. Receiving a stable proton current of ~1.3 mA, SINQ is presently the most powerful accelerator-driven facility worldwide. Besides the primary designation of SINQ to serve as user facility for neutron scattering and neutron imaging, PSI seeks to play a leading role in the development of the facility, focusing on spallation targets and materials research for high-dose radiation environments. MEGAPIE (Megawatt Pilot Experiment) is a joint initiative of six European research institutions, plus EU, JEA (Japan), DOE (USA), and KAERI (Korea) to design, build, operate and explore a liquid lead-bismuth spallation target for 1 MW of beam power [1,2].

After the integration of the target into the SINQ infrastructure in the first half of 2006 the target was irradiated by protons for the very first time on August 14, 2006 (Figure 1). Three days after the successful start-up the proton current already could be increased stepwise to the full beam power of 700 kW (1.2 mA). One week after the first irradiation the normal user operation was started and was continued without major problems until the normal annual winter shutdown starting on December 21, 2006. During that period the proton current could be increased to 1.35 mA and the MEGAPIE target received a total charge of 2796 mAh. Taking into account the complexity of the MEGAPIE system the overall availability of SINQ was again at a very satisfactory level of 95%.

Of course, the neutron flux of MEGAPIE in relation to the previously operated solid lead target was of particular interest. Based on earlier Monte Carlo simulations the liquid metal target was expected to provide a 40% increase in neutron flux

(at identical current). Initial measurements at selected instruments confirmed an increase in neutron flux: while the powder diffractometer HRPT at the thermal beam port reported 41%, very close to the prediction, the SANS-I instrument at the cold guide quoted a flux increase as high as 70 to 80% (see Figure 2). Meanwhile gold foil activation measurements have confirmed flux increases between 80 and 85% at both, a thermal beam port (NEUTRA) and a cold beam port (ICON), and 70% at sector 80 (thermal water scatterer). Revised calculations with more detailed target and moderator geometry reproduce these results.

The stable and reliable operation of the MEGAPIE target together with the tremendous neutron flux gain of 80% strongly emphasizes the wish of the user community to permanently install a liquid metal target. A project to evaluate this option has already been started. In 2007 SINQ will be operated as planned with an upgraded solid lead target, for which a moderate flux increase compared to the previous solid targets is expected.

Heavy use by Swiss universities

The installation of MEGAPIE caused an extended SINQ shutdown in 2006. The remaining time for the user operation corresponded to approximately 50% of the usual period but the higher neutron flux could partially compensate for that.

Throughout the year 260 experiments were performed on the 11 diffractive and the 2 imaging instruments at SINQ. Those 13 instruments delivered a total of 1020 experimental days and another 65 for development and commissioning. The average duration of an experiment at SINQ in 2006 was four days.



Figure 1: First beam on MEGAPIE, closely watched in the control room.

Again, the number of users was very high: the PSI user office counted 328 visits. As some scientists performed more than one experiment per year – e.g. in the course of a running long term project at SINQ – the number of individual visitors amounted to 259. The user community at SINQ is very international: users from eighteen different countries performed neutron scattering and imaging experiments here in 2006. Approximately, one quarter of the beam time was used by PSI scientists, another 30% by users from Swiss universities and

about a third was used by scientists from EU countries. The largest foreign user community came again from Germany (14%) followed by Denmark (7%) and United Kingdom (6%), 9% of the users came from Russia, Asia and the United States.

New record proposal submissions

In 2006 347 new SINQ proposals were submitted, 50% more than the previous annual record of 213. That number impressively demonstrates the interest of the user community in Swiss neutrons (Figure 3). Already in 2006 the instruments were overbooked by a factor 2.9 on average. Due to the large number of new proposals the overbooking will be at least comparable in 2007.

The main reason for the strong request is naturally the quality of the instruments, of the infrastructure – especially the sample environment and of the technical and scientific support provided by the PSI staff. Furthermore, the EU access programme NMI3 plays a major role in making SINQ attractive for the users: in 2006 another 22 projects were supported by travel and subsistence funds and a total of 112 days of access

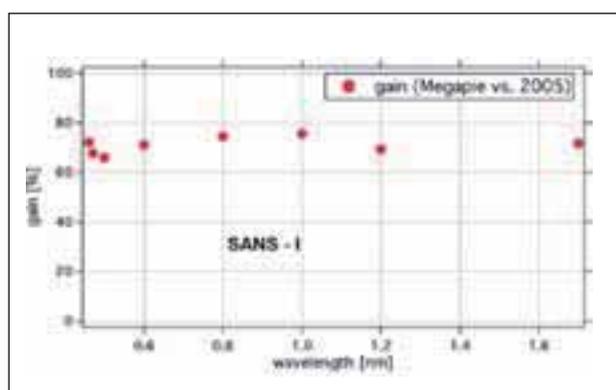


Figure 2: Flux gain caused by MEGAPIE at the SANS-I instrument as a function of neutron wavelength.

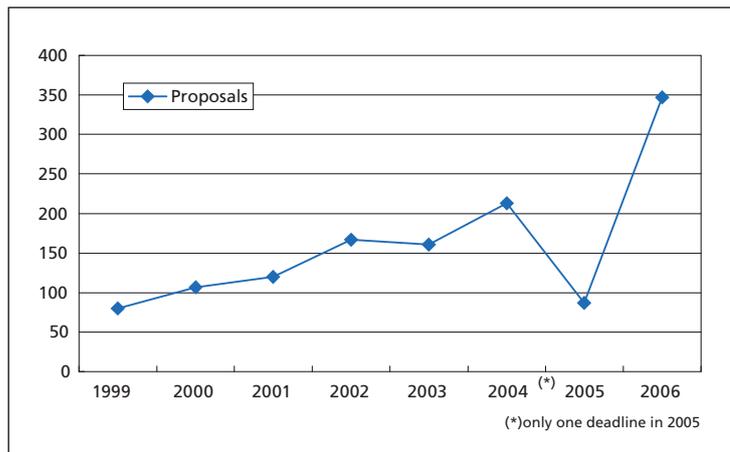


Figure 3: **History of the submission of new SINQ proposals over the last years.**

were delivered to users from eligible countries within the programme. So the participation of SINQ (and the other PSI user facilities) in the successor programme within the EU Seventh Framework Programme (FP7) will be of high importance.

A new user instrument is available: MARS

In 2006 a new SINQ instrument was commissioned: on October 14 MARS saw its first neutrons. Ten days later the first spectrum could be taken. MARS is a backscattering spectrometer that extends the experimental range of the SINQ instruments towards higher resolution and beyond the limits of the time-of-flight spectrometer FOCUS and the cold neutron triple-

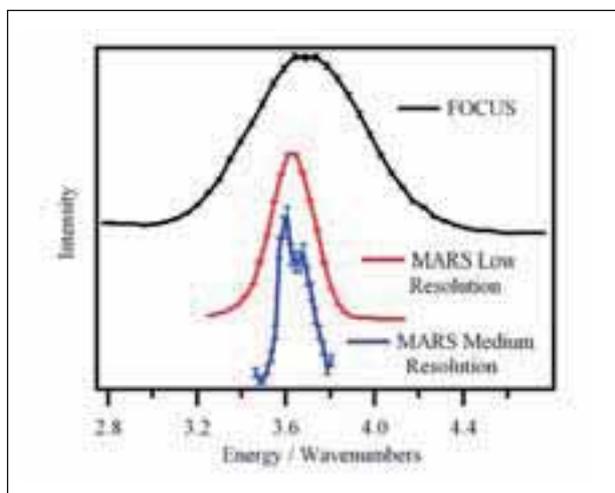


Figure 4: **One of the first spectra obtained on the new backscattering device MARS demonstrating the higher energy resolution compared to the FOCUS spectrometer. The data were obtained on an organic molecule of the Guanidinium family.**

axis instruments TASP and RITA-II. The instrument makes use of a pulsed polychromatic neutron beam tailored by five disc choppers. The secondary branch of the instrument consists of 10 mobile analyzers equipped with mica (phlogopite) crystals. The energy resolution ΔE can be tuned between 1 and 170 μeV .

Figure 4 shows one of the first spectra obtained on MARS: the data were taken on an organic molecule sample that had previously been studied on FOCUS. The comparison shows the gain in energy resolution to demonstrate the complementarity to the FOCUS spectrometer.

2007: Happy birthday SINQ !

2007 is the 10th year of full user operation at SINQ. More than 2000 experiments have been performed during that time and almost 10,000 instrument days have been delivered. On the occasion of the 10th anniversary a scientific colloquium (September 21, 2007) and a public visitors' day ('Day of the neutrons', October 28) will be organized.

References:

- [1] G. S. Bauer, M. Salvatore, G. Heusener, J. Nucl. Mater. 296 (2001) 17.
- [2] F. Gröschel, A. Cadiou, S. Dementjev, M. Dubs, C. Fazio, T. Kirchner, Ch. Latge, P. Ming, K. Thomsen and W. Wagner, "The MEGAPIE Project Status Update – High Power Liquid Metal Spallation Target", Proc. ICANS-XVII, International Collaboration on Advanced Neutron Sources, Santa Fe, NM, LA-UR-06-3904 (2006) 590.

Figure 5: **Set-up of the MEGAPIE experiment, a project involving 170 scientists and technicians from 9 partner institutes.**
(Photo: Knud Thomsen)



Swiss Muon Source S μ S

Dierk Herlach, *Laboratory for Muon Spin Spectroscopy*

The year 2006 was a very good year for μ SR at PSI in many ways. Two new instruments, the low-energy muon beam and apparatus (LEM) and the new GPD with extended high-pressure capability, were intensively used. The scientific output generated by PSI scientists and a strong international user community, benefiting from the top quality S μ S instruments, reached a new qualitative and quantitative high.

Successful operation of new instruments

In 2006 the new low energy muon (LEM) beam and apparatus (Figure 1) was fully operational for users. By providing a very powerful tool - depth resolved μ SR on the nanometre scale [1] - this worldwide unique facility significantly strengthens the leading position of PSI in the field of materials research on thin films, multilayers and interfaces. The large demand for beam time (almost twice the available) led to a dense, high quality research programme covering a wide variety of topical subjects. Based on scientific quality of the proposals and

expertise of the proposing teams, fourteen out of twenty-one projects have got beam time.

Another highlight was the set-up and successful operation of a new decay-channel μ SR facility, which replaced the oldest bulk μ SR instrument, GPD. The new instrument is particularly suited for high pressure experiments and equipped with modern sample environment covering a temperature range of 240 mK to 500 K, magnetic fields up to 0.66 T, and pressures up to 2.5 GPa.

Userlab

On the 6 S μ S instruments, a total of 597 beam days were delivered to 134 experiments of external and internal research groups, benefiting over 200 scientists from 25 countries. About 20% of the beam time was delivered to 24 projects supported within the European access contract NMI3, of which 48 users (24 receiving T&S funding) from 10 countries benefited.

High quality science output

In 2006, a total of 81 articles (of which 59 with LMU authors) were published in peer-reviewed journals. Among those, there is a significant proportion of high-ranking journals such as Physical Review Letters (9 articles, of which 8 with LMU authors), Nature Materials (1, with NUM author) Physical Review B (11, 7 with LMU authors), Journal of Physics, Condensed Matter (4, 3), and Physical Chemistry Chemical Physics (1,1).

References

[1] <http://lmu.web.psi.ch/lem/index.html> and references therein.



Figure 1: The new LEM facility at the μ E4 beamline.

The PSI/ETH Tandem accelerator facilities

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The PSI/ETH Laboratory for Ion Beam Physics provides access to a wide variety of ion beam techniques. In 2006 we had three accelerators in operation. The 6 MV EN Tandem was running for more than 3100 hours. About 73 % of the beam time was used for AMS, 19 % for materials sciences and only 8 % for conditioning. The two other AMS systems, Tandy and MICADAS, were predominantly used for experimental AMS work. Developments for a gas feed ion source and experiments to improve identification techniques of low-energetic heavy ions have been made. The Tandy system was used for routine operation of ^{41}Ca , ^{129}I and Pu.

Last year was the most successful operational year of our AMS laboratory in the past 25 years. Approximately 7000 samples were analyzed for the radionuclides ^{10}Be , ^{14}C , ^{26}Al , ^{36}Cl , ^{41}Ca , ^{129}I and Pu, about 2000 samples more than we usually analyze per year. This has several reasons: (1) a special effort has been made for the Antarctic ice core EDML with ^{10}Be and ^{36}Cl measurements. (2) We have increased the number of ^{129}I analyses at the Tandy. In particular, the influence of the North Sea to the transport of ^{129}I released into the environment from European nuclear fuel reprocessing plants has been investigated. The progress made with the measurement procedures of ^{129}I allowed the vast majority of these analyses to be performed in unattended operation mode.

(3) Routine operation of ^{14}C analyses has started at the MICADAS system. Here, the direct measurements of gaseous CO_2 samples have enabled a tremendous progress in the analysis of very small samples. It has been demonstrated that for samples as small as only a few micrograms reliable $^{14}\text{C}/^{12}\text{C}$ measurements can be performed and contamination problems which usually limit the graphitization procedure of very small samples, can be avoided. To automate the combustion process we have bought an elemental analyzer. The online coupling to the gas ion source is under development.

Biomedical applications

Biomedical AMS applications have been continued with ^{41}Ca tracer studies to investigate calcium metabolism in connection with osteoporosis disease. We could demonstrate that our

compact Tandy system is well suited for such investigations and a new ^{41}Ca study is planned with more than 1000 measurements over the next two years. To advance the AMS in life sciences we have started collaborating with Vitalea Science with the aim of building the most advanced AMS system for biomedical applications. The novel system is under construction and first beam tests are expected in 2007.

Materials science activities account for about 19 % of the total beam time on the EN accelerator. About one third of this beam time is used for our own research projects. Close to 60 % of all projects are in collaboration with groups at ETH, PSI and other Swiss or European research institutions. Approximately 10 % of the beam time is used for service measurements for Swiss industry.

EN Tandem Accelerator Operation Hours			
AMS	2004	2005	2006
Be-10	855	738	978
C-14	805	804	700
Al-26	102	33	126
Cl-36	160	265	472
Heavier Elements	136		
MS			
Materials Science	490	438	422
SSIMS	96	42	159
Maintenance			
Conditioning/Tests	424	428	259
Total	3068	2748	3116

Table 1: **Beam time statistics 2004-2006. The measurement program of ^{41}Ca , ^{129}I and Pu has been moved to the Tandy AMS system.**

Operation and development of the Proton Accelerator complex in 2006

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For the major part of the year the proton accelerator facility has shown an availability of more than 90%. Due to the stable operation and the small number of beam trips, the MEGAPIE neutron production target could be successfully put into operation in the second half of the year. The integrated charge on target E was 7.9 Ah and 2.8 Ah on the MEGAPIE target. Technical highlights of 2006 include the commissioning of a new buncher system for the Injector II, improvements of the electrostatic injection device in the Ring cyclotron and the successful operation of a modified target E with longer lifetime. Several advanced interlock systems were installed and commissioned to ensure a safe operation of the MEGAPIE liquid-metal target.

Operation

Up to week thirty-four the MEGAPIE target was still in preparation and the beam was sent to a beam dump. During this period the production current amounted to 1.4-1.6 mA, depending on the thickness of target E (1.6 with the 6 cm target and 1.4 with the 4 cm target). After the installation of the MEGAPIE target, the beam current could be increased again to the routine beam intensity of 1.9-2 mA. Due to initial operation on beam dump with reduced intensity, the delivered integrated charge has decreased as compared to the previous

years. Statistics of the 2006 production period are shown in Figure 1. The beginning of the production period was heavily perturbed by high voltage breakdowns of the electrostatic injection element (EIC). Over four weeks the phenomena were studied and several modifications were made to the electrostatic device (see section on the EIC). Another major incident in week 35 was a water leak into the vacuum at the Ring extraction magnet, causing an interruption of more than 24 hours, so that the availability in that week dropped to 70%. The reduced availability in the weeks 39 to 41 was mainly caused by repeated damage to the fibre optical cables, inter-

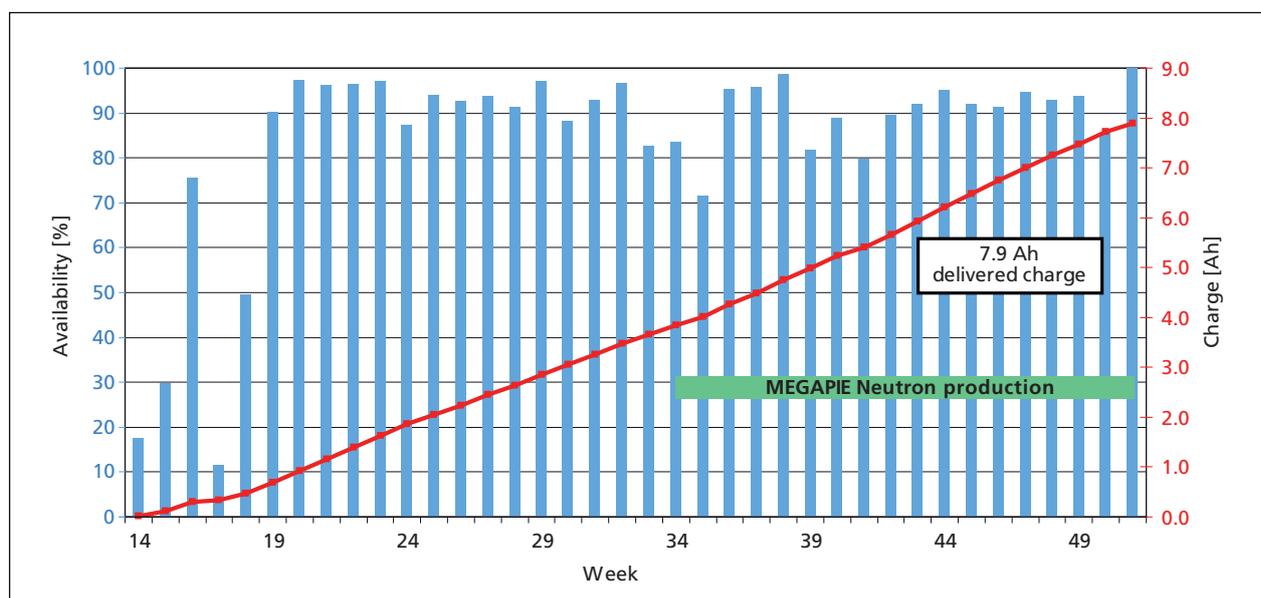


Figure 1: Operation of the Proton Accelerator: availability and delivered charge.

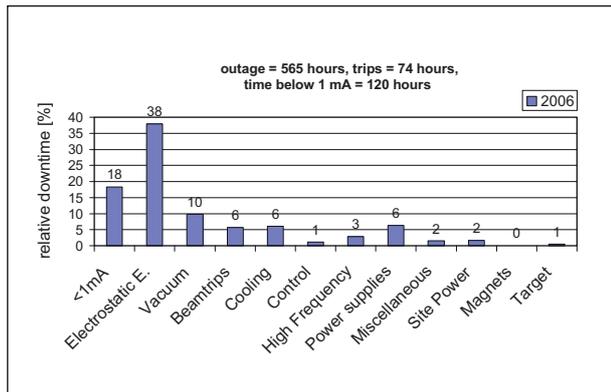


Figure 2: Sources of downtime.

facing devices on the high voltage (810 kV) platform of the Cockcroft-Walton with the accelerator control system. The ion source and the first beamline elements are situated on this platform. The damage to the fibre optics could only be eliminated after reinstalling appropriate fibres, suited for high voltage purposes. In week 35, the beam was sent to the new liquid-metal SINQ target (MEGAPIE). From then on, the beam current of the facility could be increased to its nominal value of about $1950 \mu\text{A}$. During this later period, no problems with the electrostatic devices in the Ring cyclotron occurred and the number of beam trips of 6500 stayed well below the limit of 10000 trips defined for that target.

The relative contributions of the various technical systems to the unscheduled downtimes in 2006 are shown in Figure 2. Except for the large single contribution originating from the failure of the electrostatic device EIC, similar failure rates have been observed in the past. The different improvements to the electrostatic devices (see below) seem to have been quite

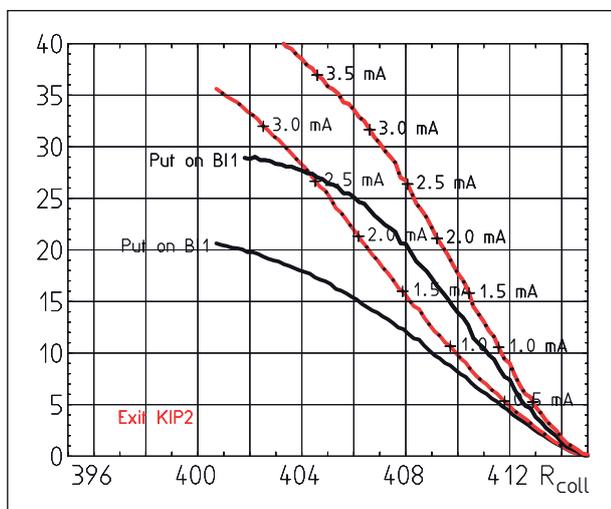


Figure 3: Fraction [%] of DC proton current passing the phase selection collimator (red) and also the set of cleaning collimators (black). The upper curves correspond to the new buncher configuration.

successful. However, the reasons for the high voltage breakdowns are still not fully understood and more studies of the phenomena are needed. Despite the fact that the CAMAC hardware is aging, the contribution of the control system to the downtime was actually small. This shows that with careful maintenance the existing hardware does not yet lead to availability problems. Nevertheless it is planned to install new hardware exclusively in VME standard and to replace the CAMAC modules stepwise over the next years.

In its 33rd year of operation the Injector I cyclotron is still used intensively. For 15 weeks proton and argon beams were provided for low energy experiments. For 11 weeks, patients were treated in the OPTIS facility. The most severe technical problems that had to be mastered were several water leaks. We plan to shut down Injector I by the end of 2007. The OPTIS treatments will be taken over by the PROSCAN facility.

Commissioning of the new buncher system

During the shutdown period 2006 the buncher system in the 870 keV injection line of PSI Injector 2 has been modified. The new buncher configuration consists of a 50 MHz main buncher followed by a low amplitude 150 MHz debunching stage. Together these two bunchers produce a long linear slope of the effective buncher voltage. The commissioning of the new buncher configuration has been performed in two steps. By means of scanning the beam intensity deposited on the beam dump BI1 as a function of the buncher phases and amplitudes, a first estimate for the appropriate buncher settings has been determined. In a second iteration, the core density of the proton beam has been maximized. To achieve this, the phase-selecting collimator KIP2 is moved across the beam profile while the fraction of current deposited on BI1 is monitored. The steepness of the slope in the resulting graph represents the local charge density across the beam. Buncher phases and amplitudes have then carefully been adjusted, accompanied by subtle tuning of selected quadrupoles in the 870 keV beamline. Figure 3 shows the increased slope achieved, in comparison to the former single buncher operation. The substantially enhanced core density allows reaching the nominal production beam intensity of 1.95 mA at a noticeably lower beam emittance. This results in reduced extraction losses in Injector II as well as in the Ring cyclotron.

Electrostatic injection channel (EIC)

The EIC is a crucial element for the injection of the 72 MeV proton beam into the 590 MeV Ring cyclotron. The electric field with a strength of 7.5 MV/m deflects the incoming beam



Figure 4: EIC with screening structure in the ring centre.

onto the orbit of the first turn in the cyclotron. The thin tungsten strips of the outer electrode allow for a small separation between the injected beam and the first turn orbit. The total voltage applied amounts to 133 kV. In an environment with the magnetic fields of the bending magnets and RF fields generated by the accelerating resonators as well as by the beam itself, it is a major challenge to avoid high-voltage breakdowns which lead to disturbing interruptions of the beam operation. A radio-frequency (RF) screening structure was proposed in response to repeated high-voltage breakdowns of the EIC. The vertical opening in the screening structure of the EIC is adapted to the 50 mm vertical opening of the collimator at the EIC entrance. A vertical and a horizontal gap with respect to the bottom and the top plate of the vacuum chamber may be recognised in Figure 4. In general the shielding plates have to be kept from any direct contact with the vacuum chamber to ensure a collision-free positioning of the EIC during operation [1].

The first shielded EIC which was installed led to a rather smooth operation of the cyclotron from May to August interrupted by only one period of frequent high voltage breakdowns that could be identified later as the consequence of a small water leak into the Ring vacuum. The second shielded EIC was in operation without any major problem for the rest of the year. Its excellent performance resulted in a new record of

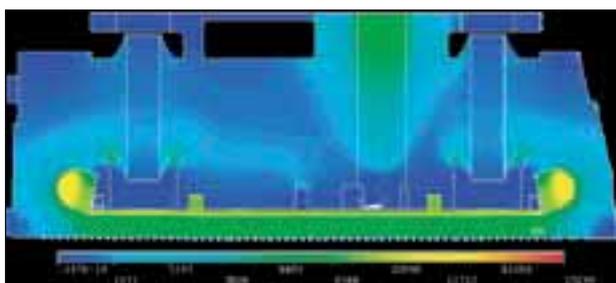


Figure 5: Vector-sum of the electrostatic field in the median plane and on the surfaces of high-voltage components. The beam passes horizontally through the even field region coloured in green.

only three voltage breakdowns per day. During the shutdown in 2007, a modified screening structure is going to be attached to the vacuum chamber in order to provide a direct electrical contact between the shielding plates and the vacuum chamber. To investigate the breakdown mechanisms the electrostatic field distribution was calculated with the ANSYS Multiphysics framework. The geometry was modelled with the ANSYS Workbench. The field analysis (Figure 5 [2]) alleviates concerns about two specific locations, namely around the contacting sphere bathing in insulating oil and near the sheath of signal cables inside the vacuum chamber. The simulation leads to the conclusion that the field values are within the dielectric strengths of all insulating components. However, in practice the breakdown voltage of a vacuum gap depends upon various factors such as pressure and content of residual gas. In addition to improving the strength of insulating media and reducing the geometrical field enhancement, establishing a clean working environment is equally important for a reliable operation of the EIC.

The field analysis establishes a quantitative base for further development. The 3D model has proven to be useful for the design of the RF screening structure, as the measurement is carried out on the model instead of radioactive components. The field distribution can be readily simulated for a modified EIC with the aim of enhancing the high voltage holding capability.

Meson production targets

The megawatt proton beam from the 590-MeV Ring accelerator is guided to two meson production targets, “M” and “E”, mounted in series, to generate intense pion and muon beams for research in particle physics and for muon-spin-resonance applications [3]. Both targets consist of radiation cooled rotating wheels from polycrystalline graphite. Target-M is 0.5 cm thick and target-E has two versions, one with 4 cm and the other with 6 cm thickness. Since 2000, the shorter target-E version with a length of 4 cm has been used. As a result, the beam current for SINQ has increased by 20% due to the lower beam losses in the target and in the subsequent beam shaping collimator. The operational lifetime of the target wheels is affected by the irradiation-induced anisotropic shrinkage of the polycrystalline graphite, which causes deformation of the shape that leads to a radial wobble.

Figure 6 shows the integrated beam current up to the point of failure for different versions of target E made from the graphite grades R6300P and R6510P, as a function of the beam intensity. For beam intensities above 1.5 mA the targets were made from R6510P, which is a more isotropic form of graphite [4]. This has resulted in a significant improvement of the

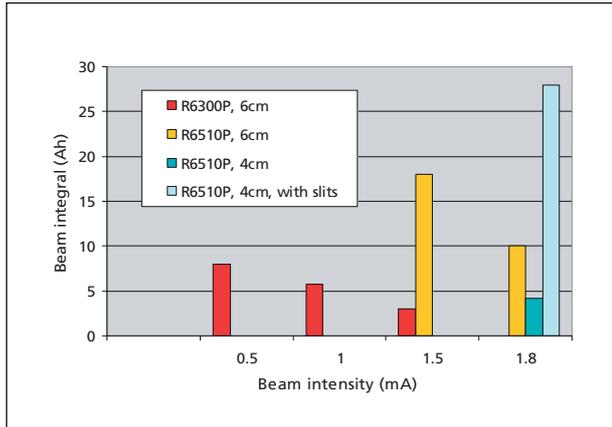


Figure 6: Achieved beam integral up to the point of failure for target wheels made from graphite grades R6300P and R6510P, as a function of beam intensity.

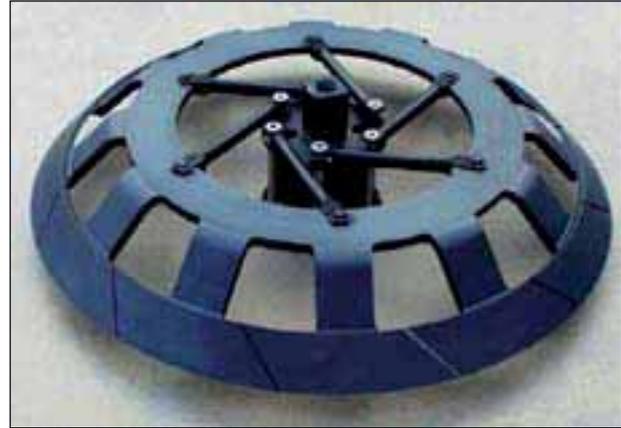


Figure 7: A new, slitted target design avoids deformation due to irradiation-induced dimensional changes of the graphite.

lifetime of the 6 cm targets, which presently reaches 10 Ah at 1.8 mA, corresponding approximately to one operational year.

For the 4 cm target the lifetime dropped to 4 Ah, corresponding to only a few months of operation. This may be a consequence of the lower stiffness. In order to increase the operational lifetime, a new design of the graphite wheel, as shown in Figure 7, has been developed. The target cone is subdivided into 12 segments separated by gaps of 1 mm at an angle of 45° to the beam direction. This allows unconstrained dimensional changes of the irradiated part of the graphite. At the normal operating temperature, the gaps in the beam direction narrow down to about 0.5 mm. With these slits the lifetime of the target increased to more than 28 Ah.

Special interlock systems for MEGAPIE

To guarantee a safe operation of the MEGAPIE liquid metal target the beam transverse density at the entrance window has to stay below a certain maximum value. The beam density is basically determined by scattering at the 4 cm graphite target E and the beam optical system which transports the beam to MEGAPIE. A triple redundant interlock system has been installed to monitor the correct scattering of the beam at target E:

- Beam current transmission monitor for the beam passage through target E.
- Slit system in the dispersive focus of the bending section below the SINQ target.
- Visual monitor for the light emitted by a glowing mesh below the SINQ target.

A quick and reliable detection of erroneous beam conditions is sufficiently guaranteed by these three independent devices.

The transmission monitor has a high resolution which allowed detecting the small current modulation that is caused by the above mentioned thin slits in the rotating target E. Main reasons for erroneous beam conditions are portions of proton beam bypassing target E or wrong quadrupole settings of the beamline to the SINQ target. Each of the three devices has a different sensitivity and response time, but each has been designed to be fast and sensitive enough to protect the MEGAPIE target from being damaged by the proton beam. Additionally to the three devices mentioned above, the settings of the last 6 quadrupole lenses and the last 2 bending magnets of the proton beamline were only allowed to be varied within limited margins in order to guarantee the correct beam transport to the MEGAPIE target. For maximum safety, the control electronics of the three devices were connected to the accelerator's run permit system (interlock system) and to the Schnelles Abschalt System (SAS) of the SINQ. In case of a faulty proton beam condition both systems turn off the proton beam. During the whole period of operating the MEGAPIE target in 2006 all systems behaved excellently and no safety glitches were detected.

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PSI-XFEL: the challenge for ultra-bright X-rays

René Bakker, Romain Ganter, Christopher Gough, Peter Ming, Marco Pedrozzi, Frédéric Le Pimpec, Jean-Yves Raguin, Fuqiang Wei, Albin Wrulich, *PSI FEL with support from the Departments of Large Research Facilities (GFA), Logistics (LOG), and Synchrotron Radiation and Nanotechnology (SYN)*

The PSI considers the construction of a Free-Electron Laser (FEL) for femto-second X-ray science as the next large-scale facility [1]. Combined with the SLS it will form the basis of an Ultrafast X-Ray Science Park for the national and international scientific community. Naturally, such an ambitious goal needs thorough preparation and, most importantly, it requires the development of new accelerator technology to pave the way towards a cost-effective and reliable design of such a future facility.

Introduction

An X-ray Free-Electron Laser (XFEL) can generate light-pulses with a selectable wavelength, a peak power of several GW, and duration of several fs. It thus forms the ideal complement to the Swiss Light Source, enabling the pursuit of revolutionary new science.

The construction and operation of a FEL is challenging. In addition, a cost-effective design, based on a moderate energy accelerator, also lacks the availability of a high-brightness electron source, and a lack in accelerating-schemes that preserve this brightness. The PSI-XFEL project looks at all aspects, i.e., development of a suitable electron source, acceleration schemes, and the layout of a future X-ray FEL facility.

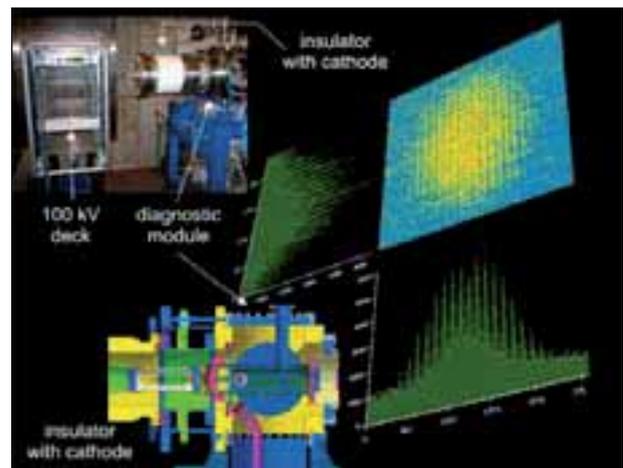


Figure 2: Measurement of the brightness of an electron beam from a field emitter array at 100 kV.

High brightness electron source

The Low Emittance Gun (LEG) project introduces new technology for the generation of ultra-bright electron-beams. LEG consists of a cathode based on field emission, a high-gradient pulsed accelerator, and a custom designed RF accelerator. Figure 1 depicts a test cathode fabricated by the Laboratory for Micro- and Nanotechnology (LMN) at PSI [2]. These all-metal arrays with pyramidal shape are designed to provide a higher average current as compared to commercial devices. The year 2006 marked a break-through of the production process, yet further R&D is needed to reach the required emission current and beam characteristics.

The 500-kV pulser shown in Figure 3 has been designed to accelerate the electrons quickly and preserve the high bright-

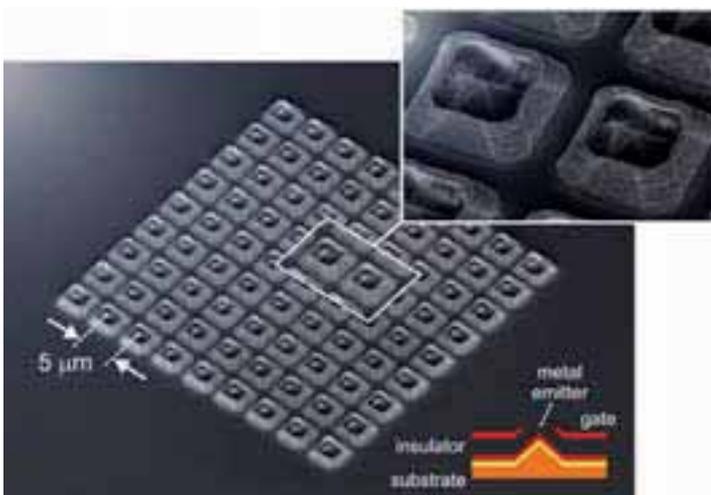


Figure 1: Field Emitter Array tests to generate ultra-bright electron beams. The devices are fabricated at the Laboratory for Micro- and Nanotechnology (LMN) at PSI [2].



Figure 3: **500 kV High Gradient Pulser installed in the LEG test bunker.**

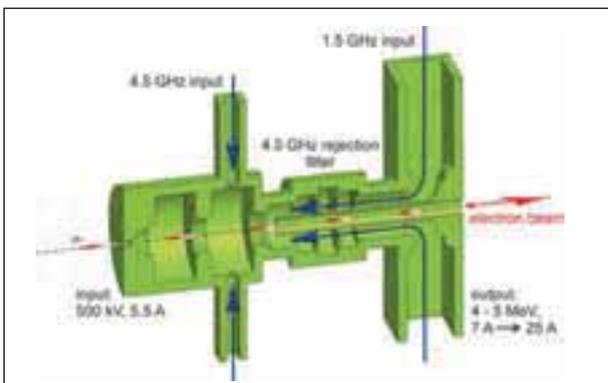


Figure 4: **The 2-cell, 2-frequency standing-wave RF cavity boosts the brightness of the electron source.**

ness. In December 2006 it reached its target voltage. First operation with beam is planned in early 2007.

At the exit of the 500-kV pulser the beam is injected into a two-frequency two-cell RF cavity (see Figure 4). The tasks of this cavity are: (1) a further increase of the beam energy up to 4 MeV, and (2) ballistic compression. The former further reduces the influence of space charge. The latter reduces the negative effects of space charge since it permits an initially low peak-current at the cathode, which is increased at higher energy. The RF design of a single frequency version of this cavity was completed at the end of 2006. Installation of this first prototype of this device is planned in the fall of 2007.

The layout of the complete assembly of LEG is presently under construction and will be located in an existing test-bunker at PSI. An overview of the infrastructure is shown in Figure 5. A high power ps laser has been introduced to trigger the emission process from the cathode. In addition the figure depicts the outline of a diagnostic section to measure the performance of the gun.

250 MeV Acceleration

At the exit of the gun the peak current is still insufficient to drive an X-ray FEL and, more important, the quality of the

beam remains sensitive to space charge. Studies of the electron beam dynamics show that the first 250 MeV of acceleration are critical. It is for this reason that the next step of the PSI-XFEL project concentrates on the design of a test accelerator for this energy range. The construction and operation are proposed for 2008 to 2011, in which period it serves as an experimental test-environment to evaluate the technological risks of high brightness beam acceleration in relation to its use as a future injector for an X-ray FEL linac system.

X-ray FEL facility

The present PSI-XFEL design is generic and used to: (1) specify the required performance parameters of the 250-MeV injector, and (2) verify the feasibility to construct a cost-effective XFEL with a medium energy accelerator. In summary the facility is driven by a 6-GeV linac and has a spectral coverage from 10 nm (124 eV) to 0.1 nm (12.4 keV) with three independent beamlines [3].

Further Information

[1] <http://fel.web.psi.ch>

[2] <http://lmn.web.psi.ch/>

[3] <http://fel.web.psi.ch/public/xfel/FEL-BR06-004-FEL-Performance.pdf>

Acknowledgements

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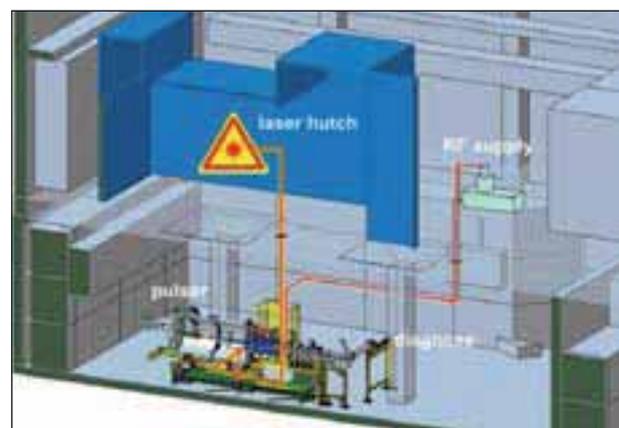


Figure 5: **Layout for the Low Emittance Gun (LEG) test facility.**



HANDY
MOLD

Technology transfer 117

118 Projects in diagnostics, pharmaceuticals, high precision mechanics, and energy technology

The portal between research and industry

The technology transfer office at PSI offers its services to enable and support the transfer of results from research to industrial applications. Through these activities, society benefits from the economic impact that results from these companies and by the availability of new products.

The motivation for such transfer and cooperation activities can emerge from the researcher who has achieved a result with a potential for commercialization, but the initiative may also begin with an enterprise that has very specific technological questions or needs for innovation.

Research cooperations with academic institutions and industry, as well as our own research, generate know-how and patents that we offer to companies for licensing. The rights of use and the compensation models vary among the technologies and their applications. Therefore the license agreements are negotiated individually according to the circumstances of the specific case. Over the last years, an average of seven license agreements per year has been signed with industrial partners, and in 2006 PSI filed patent applications for 42 inventions.

The R&D activities of companies are the sources for new products and therefore have a high strategic significance. A successful transfer requires sensitivity, mutual respect and appreciation for the environment of the partners. Within this individual-related environment, the technology transfer office supports transfer projects and continuously searches for new approaches to join the interests and potential of both industry and PSI.

**Nanotechnology with
plastics: injection moulding
machine in joint lab of PSI /
University of Applied Sciences
Northwestern Switzerland
in Windisch.**

(Photo: H.R. Bramaz)

An invention for new tumour diagnostics

Thomas L. Mindt, Harriet Struthers, Roger Schibli, *Centre for Radiopharmaceutical Science, PSI-ETHZ-USZ*

The radiolabelling of biologically active molecules has become an indispensable tool for the assessment of novel drug candidates in animals and humans. To keep pace with the growing number of new lead compounds and drug targets, innovative and efficient methodologies are needed for the incorporation of radionuclides into molecules of interest. Using ‘click chemistry’ we have shown that the numbers of synthetic steps necessary for the modification of tumour-targeting molecules can be significantly reduced. This approach allows a more efficient and rapid development of novel radioactive tracers useful for diagnosis and therapy.

A prime goal of the Centre for Radiopharmaceutical Science at PSI is the development of new diagnostic and therapeutic tumour targeting radiopharmaceuticals for potential use in nuclear medicine. These efforts require the constant improvement of methodologies in order to incorporate radionuclides with optimal decay characteristics. The single photon emitting radionuclide ^{99m}Tc -technetium is readily available at low costs and possesses excellent decay properties for diagnosis. Therefore, it is of highest interest for the radiopharmaceutical industry to develop novel tracers which comprise this radionuclide. A few years ago at PSI we invented a kit preparation for the radio-labelling precursor $[\text{M}(\text{OH}_2)_3(\text{CO})_3]^+$; ($\text{M} = ^{99m}\text{Tc}, ^{188}\text{Re}$) [1]. This precursor has recently become commercially available (IsoLink™, Mallinckrodt-Tyco). However, the incorporation of suitable metal chelators for this precursor into molecules of interest remained a synthetic challenge because it requires multiple-step syntheses due to cross-reactivity with other chemical groups.

Description of invention

We essentially solved the problems mentioned above by employing Sharpless’ ‘click chemistry’ (the copper (I)-catalysed

[3 + 2] cycloadditions between organic azides and acetylenes forming a stable 1,2,3-triazole linkage [2]). Click chemistry is particularly valuable because it is efficient, selective and devoid of cross reactions. No reported examples of 1,2,3-triazole metal chelators useful for Tc and Re existed (Figure 1).

We proved the viability and versatility of a ‘click-to-chelate’ approach using various classes of biomolecules (e.g. peptides and vitamins). Our experiments have demonstrated that this methodology allows not only the design of novel polyfunctional metal chelates but more intriguing it solves the problems associated with coupling metal chelates to biomolecules [3].

Future scope of invention

Selection and preparation of an optimal novel radiotracer can now be rapidly made by structural variation of the metal chelator. Implementation of this strategy into a high-throughput system is currently the subject of investigation in our laboratories. Such aspects are of great interest to the (radio) pharmaceutical industry in their goal of optimizing the drug development process.

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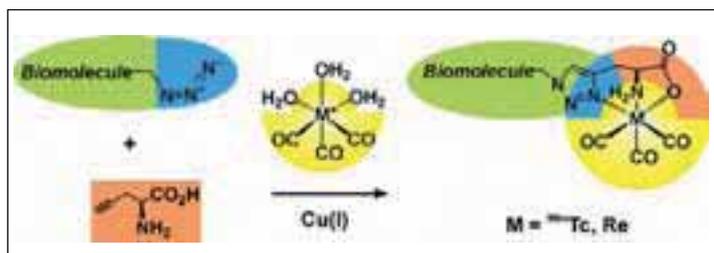


Figure 1: **Novel functionalization and radiolabelling strategy of organic molecules via ‘click chemistry’.**

Neutron imaging of polymer electrolyte fuel cells: a powerful tool for science and industry

Pierre Boillat, Denis Kramer, *Electrochemistry Laboratory, PSI*; Eberhard Lehmann, *Neutron Imaging and Activation Group, PSI*; Günther G. Scherer, *Electrochemistry Laboratory, PSI*

Water management is widely recognized as an important challenge for the development of the polymer electrolyte fuel cell (PEFC) technology. A very powerful and non-intrusive technique to detect and quantify water in fuel cells is neutron radiography, developed at PSI in close collaboration between the Electrochemistry Laboratory and the Neutron Imaging Group. For several years, our industrial partners have profited from this unique in situ method to obtain an unprecedented insight into their fuel cells.

The presence of liquid water in polymer electrolyte fuel cells (PEFC) has both beneficial and detrimental effects: the polymer membrane needs to be well hydrated to fulfill its function as a proton conductor. However, an excess of liquid water can reduce the access of reactant gases to the active sites. For this reason, the ability to visualize liquid water inside a working fuel cell is highly valuable.

A non-invasive method

Among the available methods, neutron radiography offers decisive advantages: the materials commonly used for the construction of fuel cells can be penetrated by the neutron beam, suppressing the need for special housing and flow field materials and thus making the method non-invasive. Moreover, water can not only be visualized but also quantified thanks to advanced image processing tools developed at PSI.

For several years, neutron radiography applied to fuel cells has been successfully performed by the Electrochemistry Laboratory in close collaboration with the Neutron Imaging group of the SINQ spallation neutron source [1]. Considerable progress was achieved in the understanding of fuel cells, the improvement of the neutron radiography method [2-3], and the combination with advanced spatially resolving electrochemical diagnostics developed in the Electrochemistry Laboratory [4].

High interest from industry

Neutron sources of sufficient intensity to perform radiography on fuel cells are facilities which cannot be transferred as is to

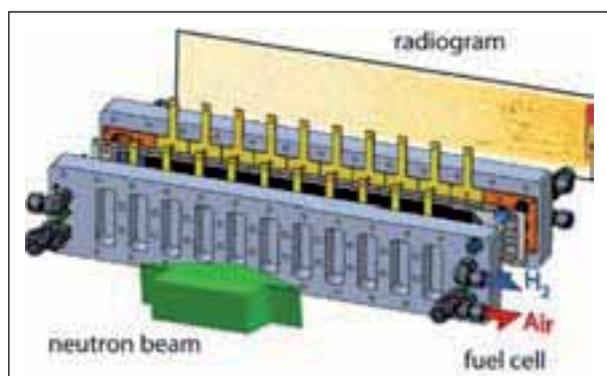


Figure 1: Neutron radiography of a fuel cell.

industry. Instead, the neutron radiography technique is transferred to industrial partners in the form of service or joint research contracts, with the measurements taking place at PSI. The infrastructure offered at PSI in terms of neutron imaging as well as fuel cell testing capabilities has gained the interest of several industrial partners. In particular, the long term collaboration with Nissan Motor Co., Ltd, has allowed the addressing of several topics of scientific and industrial interest.

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The next generation of accelerator mass spectrometry for bioscience and microdosing

Hans-Arno Synal, Tim Schulze-König, Martin Suter, *Research Department Particles and Matter, PSI, and Institute of Particle Physics, ETH Zurich*

To make available the most advanced AMS technology to Bioscience, PSI and Vitalea Science have entered into a collaborative agreement to build a novel AMS instrument. PSI will provide expertise for design and construction of the new instrument and Vitalea Science will provide expertise and experience as a biomedical AMS service provider. The new instrument is under construction and initial beam tests are planned for mid-2007. PSI has an interest in the know-how gained from this collaboration and its scientific exploitation, a long-term operation of the new instrument by PSI is not envisioned.

Although accelerator mass spectrometry (AMS) technology was developed in the late 1970s, it has taken many years to see its introduction into biomedical research. Reasons for this include the size, complexity, and the costs of the original instrumentation as well as the specialist nature of both the equipment and personnel to run it. However, the advantages of AMS over traditional methods are tremendous [1]. With AMS, radioactive doses involved are 1,000- to 10,000-fold reduced and not much different from natural dose levels. Radiological and ethical aspects will no longer limit the type of experiments and clinical studies and it is expected that AMS will, in future, become a key technology in these research fields.

A tabletop AMS system for bioscience

Driven by the developments made at the PSI/ETH AMS group [2] to utilize low charge state ion beams for the detection of long-lived radionuclides at natural levels, a new generation of AMS spectrometers became available to the AMS user community. In a further development we could demonstrate that, particularly for radiocarbon AMS, systems can be built which will not use conventional accelerator technology, but a vacuum insulated high voltage platform charged by a commercial high voltage power supply [3]. This new concept has implications for life science applications and it can be anticipated that technical and analytical restrictions which up to now have impeded a widespread usage of AMS technology can soon be overcome.

Based on these ideas, PSI has started to design a new AMS instrument optimized to the needs of biomedical radiocarbon tracer studies. Our aim is to demonstrate that the latest de-

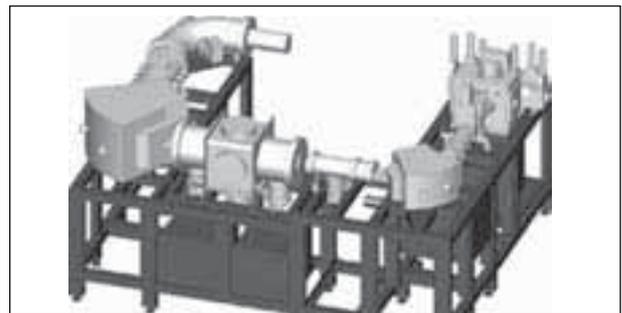


Figure 1: **Design view of the new BioMICADAS AMS system. The footprint of the system is only 2.5x3 m². The system will have no open high-voltage potentials and all essential system components are accessible during operation. It will be fully automated, easy to tune and operate.**

velopments in AMS technology are capable of fulfilling the requirements of biomedical research.

In parallel with systematic instrumental and technical developments we have initiated a scientific partnership with Vitalea Science, Davis, CA, USA, one of three companies who have a licence to perform commercial radiocarbon AMS micro-dose studies.

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SO_x traps – manganese oxides help to protect automotive catalysts

Oliver Kröcher, Kirill Tikhomirov, Martin Elsener, *Combustion Research Laboratory, PSI*; Alexander Wokaun, *Research Department General Energy, PSI*

One of the major challenges in the development of automotive catalysts is that sulphur oxides (SO_x) cause the catalysts to deactivate therefore restricting the range of components to sulphur-insensitive chemical elements and compounds. One way to overcome this problem is the application of an SO_x trap upstream of the catalyst. Manganese oxide proved to be an ideal material for this purpose. Not only is it a cheap material, but it is capable of quantitative absorption of SO₂ from hot exhaust gases.

Nitrogen oxide storage and reduction (NSR) catalysts are the most prominent example of automotive catalysts that are significantly deactivated even by low concentrations of SO₂ and SO₃ in the exhaust gas. Some catalysts can be regenerated periodically at elevated temperatures, but this implies a fuel penalty and exposes the catalyst to thermal stress. A different approach to cope with the sulphur problem is the introduction of an SO_x trap upstream of the exhaust gas after treatment catalyst. Such an SO_x storage device may be disposed and replaced when it reaches its maximum storage capacity. This is a promising concept, but finding a material which meets all the following requirements seems to be very challenging. Both storage capacity and storage rate have to be high enough at all engine operating conditions to provide almost complete removal of sulphur for the whole lifetime of the trap. Sulphur must be stored stably in order to prevent its unintentional release, which would result in poisoning of the downstream catalyst system. Finally, a low price is an important criteria for the consideration of SO_x storage devices for future vehicle applications.

Besides the insufficient performance most of the proposed materials failed due to their high price. Surprisingly, we found manganese oxide (MnO_x) to be a simple and cheap material for the storage of SO_x, which seems to be superior to all previously described specially tailored SO_x traps.

The key features of this promising material have been investigated in detail. The manganese oxide prepared at PSI shows an almost constant SO_x storage efficiency in contrast to commercial manganese oxide, whose efficiency is steadily decreasing during the storage process. The superior performance of the PSI material results from its labile crystal structure, which is easily converted during sulphatization resulting in a much smaller diffusion resistance.

The storage efficiency stays the same for particle sizes within a broad range, i.e. SO_x storage depends only on the amount of material, which facilitates broad design variability for real exhaust gas aftertreatment systems – from simple coatings to complicated geometrical moldings.

The storage capacity of the material can be fully exploited also under real conditions. Thereby, the storage process is not influenced by CO₂ and NO, two less reactive components of automotive exhaust gas.

SO₂ and SO₃ are stored with the same efficiency. Unlike many other storage materials, the SO₂ storage over MnO_x does not require the preliminary oxidation of SO₂ to SO₃ over an expensive platinum catalyst.

These results show that it is possible to efficiently remove sulphur from exhaust gases with a relatively simple and cheap material. A preliminary scale-up of the data obtained from powder experiments revealed a maximum space velocity of 15,000 h⁻¹ for a coated monolith if quantitative SO_x absorption is required. This space velocity is too small for a practical application so far, but alternative reactor designs are conceivable providing much more storage material than a coated monolith.

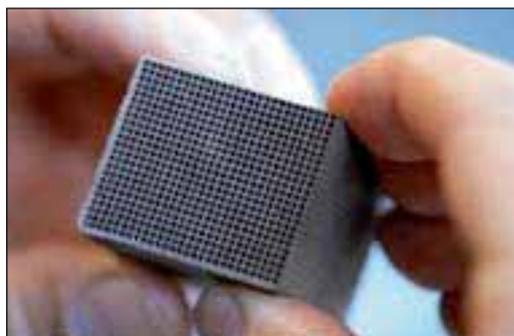


Figure 1: Manganese oxide, a promising material.

MYTHEN X-ray detectors

Anna Bergamaschi, Bernd Schmitt, Markus Naef, Hermann Rickert, Raphael Baldinger, Fabia Gozzo, Bruce Patterson, *PSI*

MYTHEN is a one-dimensional detector designed for powder diffraction experiments at the SLS [1]. Due to its massively parallel detection of X-rays and fast readout, it allows the performance of time resolved or dose-critical measurements in seconds or less, instead of minutes or hours as with traditional analyzer systems. A system covering 60 degrees is available for users' operation at the material science beamline and has made time-resolved powder diffraction experiments possible for the first time [2] over a large angular range and with good angular resolution. It will soon be replaced by a newly upgraded version of the system, which allows measurements on a time scale of milliseconds, instead of seconds, and gives improved performances at low energies. The system is suitable also for several other X-ray applications.

The MYTHEN detector is a one-dimensional microstrip detector optimized for time resolved powder diffraction experiments.

The detector operates in single photon counting mode, that is, each incoming photon is counted. The properties of the MYTHEN detector are:

- Dynamic range of 24 Bit
- Highest sensitivity in the energy range of 5 – 15 keV
- Read-out times of about 0.3 ms
- Spatial resolution 50 μm

The high dynamic range enables the recording of very strong and very weak X-ray signals with high precision. The short readout time allows the study of dynamic processes.

A setup consisting of a single module with 1280 channels and its readout system is available. It can run on any Linux PC. The control is performed by a user friendly graphic interface. The system can be operated with a frame rate up to 200 Hz. The single module setup is very compact and needs only a connection to the Ethernet and to the electric network.

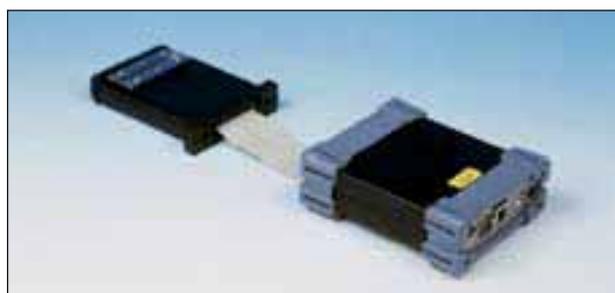


Figure 1: **The MYTHEN single module setup. The active width of the detector is 64 mm.**

The components of the detectors are fabricated by Swiss companies, except for the CMOS chips and the sensors. Fabrication and assembly of the detectors is partially out-sourced to nearby companies.

A 24 module system will be installed at the material science beamline at the SLS in order to acquire powder diffraction patterns covering 120 degrees.

The main applications are:

- X-ray powder diffraction
- Imaging
- Small angle X-ray scattering (SAXS)
- Time resolved experiments

Test measurements have been successfully performed for all these applications at the SLS and at other synchrotron radiation facilities.

The system is particularly suitable for synchrotron radiation experiments, which are extremely challenging because of the high X-ray intensity.

Several synchrotron radiation facilities have shown their interest in buying the MYTHEN detector for various applications. The detector is also suitable for laboratory diffractometers, where the high spatial resolution and the photon counting capability enhance the capabilities of such systems. Industrial contacts have been established with major companies in the field of laboratory diffractometers.

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High precision mechanics for research and industry

Haimo Joehri, *Department of Mechanical Engineering Sciences, PSI*

The Department of Mechanical Engineering Sciences at PSI has the task of developing many types of machinery systems and components that must work in an ultra-high vacuum. The demand for motion precisions better than 0.1 micrometre in this environment is solved with flexures that are free from friction and backlash. The nanoconverter is a linear gearbox for nanomotion. The gimbal-mount is a system for the positioning of optical components with ultra-high precision. Both systems are constructed with few parts. The main advantages are: cost-effective manufacturing, very high precision, free of mechanical wear, easy to manipulate and maintenance-free.

Nanoconverter

The nanoconverter allows the use of conventional commercial actuators for movements with nanometric precision by means of a perfect linear downscaling of the movement amplitude by a large factor.

The whole part is manufactured as one piece including the following functions: mounting frame, input stage, intermediate parallel spring stage and output stage.

The gear reduction results from the differential shortening of the converter blade with respect to the blades of the parallel spring stage. Those blades are deformed in a natural S shape. With that arrangement, two parabolic motions are subtracted. It can be mathematically derived that the resulting motion is a linear gear reduction. The gear transmission ratio can be defined from 1:20 to 1:1000.

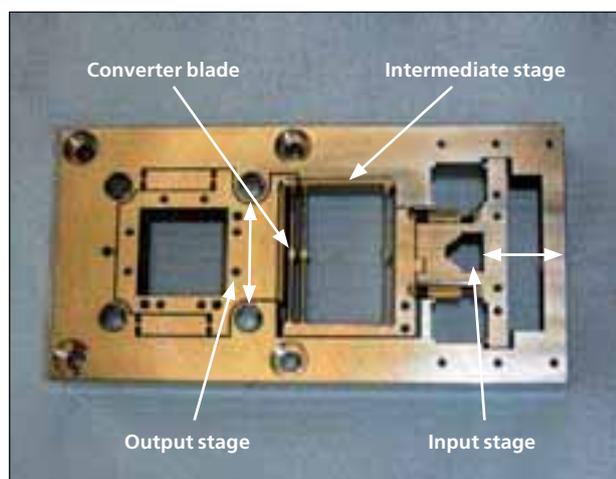


Figure 1: **The Nanoconverter allows motions accurate to less than 0.1 micrometre.**

Gimbal-mount

A mirror can be fixed on the gimbal-mount in such a way, that it is positioned in the same plane with two swivelling axis and both axes are completely independent.

The gimbal-mount has two elastic pivot bearings which operate without any slack in the system. The positioning of the angle is done by a stroke with travelling mandrels. The complete cardan joint is manufactured in one piece.



Figure 2: **The Gimbal mount can position optical devices with high precision.**

Pharmaceutical applications of X-ray powder diffraction at the SLS

Fabia Gozzo, Dominik Meister, Michael Lange, Bruce Patterson and Bernd Schmitt, *Research Department Synchrotron Radiation and Nanotechnology, PSI*

X-Ray powder diffraction (XRPD) has become a predominant analytical tool in pharmaceutical applications for the characterization of a new drug during all phases of its life cycle (discovery, development and commercial manufacturing). The combination of high-resolution and fast-acquisition times available at synchrotron facilities is pushing the development of XRPD in the field of pharmaceuticals. Besides technical excellence, at the SLS Powder Diffraction Station we emphasize professionalism, reliability and confidentiality.

Because each crystal structure generates a unique powder diffraction pattern, the traditional application of XRPD allows the identification, or *fingerprinting*, of crystalline phases, after the structure has been determined using single crystals [1]. In recent years, the development of new powerful computational methods and high-resolution and fast X-ray detectors have opened new horizons to XRPD.

Pharmaceutical research is undoubtedly a field where XRPD is quickly becoming a key analytical technique applicable during all phases of the life cycle of a drug, that is, discovery, development and commercial manufacture. Furthermore, XRPD has proved to be extremely valuable for protecting intellectual property during the patent lifetime of a drug [2].

The powder diffractometer (PD) at the SLS materials science (MS) beamline combines ultra-high-resolution (down to 0.003° in 2θ) and ultra-fast (down to a few seconds for a full diffraction pattern) capabilities and has proved to be a valuable tool for the pharmaceutical industry. This is particularly true when laboratory X-ray diffractometers reach their limits, e.g. for high-resolution data for crystal structure solution, weakly-diffracting organics with amorphous components, polymorphic purity and/or additional crystalline phases analysis, powder profiles from substances available only in a few milligrams, dilute nano-crystal suspensions or highly toxic or reactive compounds. Figure 1 shows powder profiles on a Cilag AG organic substance with conventional sources (1-2) and at the SLS PD station (3). The low background, high counting-rate and resolution of the synchrotron data make them extremely valuable.

For proprietary access to the SLS, industrial users are charged for the beam time (for information, contact philipp.dietrich@psi.ch). Fast access and purchasing of only small fractions of an 8-hours beam time shift have been successfully imple-

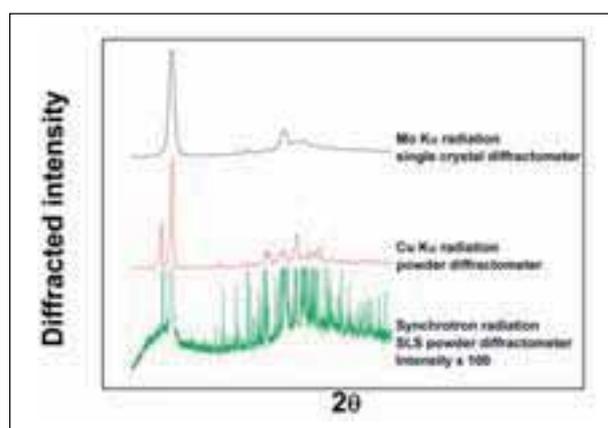


Figure 1: Powder diffraction profiles of an organic substance with texture effect (courtesy of Thomas Laube and Winfried Fiedler, Cilag AG).

mented. Upon request, measurements are entirely performed by the beamline staff and an accurate calibration of the 2θ angles and the photon energy is always supplied together with technical support, scientific advice, professionalism, confidentiality and respect for deadlines. The contact with industrial users has been so far a truly win-win experience, often stimulating improvements at the beamline.

Acknowledgement

We thank Nathaniel Finney for helpful discussions.

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Neutron diffraction for industrial applications at SINQ

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Neutron diffraction is a unique technique for investigating the chemical and magnetic structure of new materials. Neutrons can easily penetrate matter, and are therefore suitable for bulk material, and they allow the use of a massive and heavy sample environment to create extreme external conditions (T,P,H). Light elements such as hydrogen or lithium can be detected in the presence of heavy elements; isotopes and the elements with close Z can be distinguished, as well as the electron magnetic moments. The strains in the bulk materials, for instance in rails or coatings, are of keen interest for industrial/technology applications.

Neutron diffraction is a state-of-the-art technique which can obtain a clear picture of the chemical structure and phase transitions, especially if light atoms or magnetic properties are the focus. Chemical reactions can be investigated in-situ. New materials are normally available first in a polycrystalline form. SINQ offers three neutron powder diffraction (NPD) instruments: HRPT (high resolution and the wide range of d-spacing allow precise structure determination), DMC (high-intensity and resolution at large d-spacing allow studying complicated magnetic structures). The high penetration of the neutrons is used at the high-resolution POLDI instrument investigating strain and stress in huge samples such as welding areas in rails or coatings of turbine blades. If single crystals are available, the single crystal diffractometer TriCS offers further possibilities.

An example of using NPD is the elucidation of the crystallographic site preference in the Laves phase of the system Ti-(Fe,Co,Ni)-Al as a profound basis for proper thermodynamic modelling as well as interpretation of physical properties [1]. Laves phases, the largest group of intermetallic compounds, enjoy widespread practical applications because of their unique functional and structural properties. In addition to magnetic, superconducting, hydrogen-storage, and tribological applications, some intermetallic Laves-phases have been developed for high-temperature structural use, such as jet aircraft engines. The atomic site parameters and atomic occupation are the key parameters affecting mechanical behaviour and other physical properties such as magnetism.

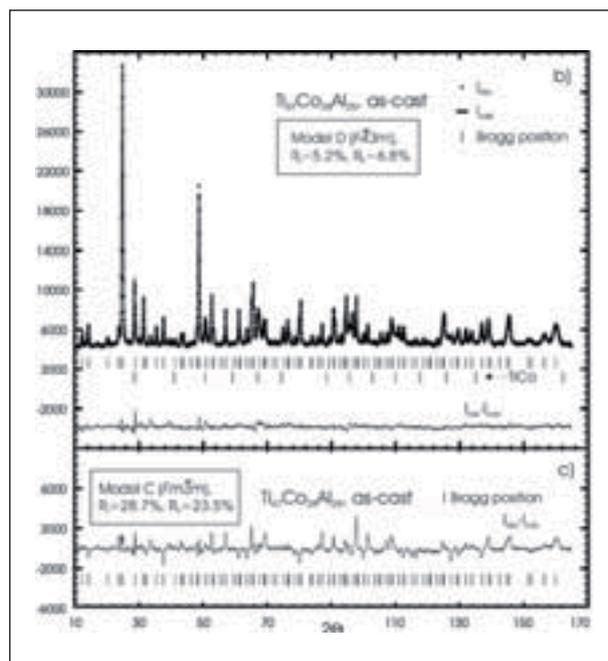


Figure 1: **The results of Rietveld profile refinement of the neutron powder intensity data for the alloy $Ti_{47}Co_{28}Al_{25}$. Despite the good agreement on the site preference obtained by X-ray diffraction analysis, the neutron data do not agree with those models (e.g. see the difference curve for model C). The model D, which split each 32f site (in S.G. Fm3m) into two 16e positions, offers options for further atomic ordering and leads to excellent agreement with the experiment.**

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Particulate matter: a breathtaking subject in winter

André Prévôt, Sönke Szidat, Rami Alfarra, Jisca Sandradewi, Silke Weimer, Urs Baltensperger,
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In January and February 2006, the highest particulate matter concentrations for many years were measured on the Swiss Plateau. The debate in the media was heated, various statistics concerning the polluters were communicated and the finger was pointed in different directions. The big question is, of course, who is responsible for these high concentrations during such winter episodes. In previous winters, but also during that 2006 episode, the Laboratory of Atmospheric Chemistry (LAC) performed new types of measurements allowing a better source attribution than previously possible. The results obtained were communicated to the public and the air pollution authorities by press releases, newspaper articles, and television reports.

The German word for particulate matter – *Feinstaub* – has only been widely known in Switzerland since the winter 2005/2006 when the concentrations exceeded the legal thresholds in northern Switzerland for weeks.

Is diesel traffic really so important?

The discussion focused initially on traffic, especially diesel trucks and diesel passenger cars. Particle filter technology is available to get rid of most of these emissions. In our analyses

in the village of Roveredo in the Mesolcina valley, however, we found that domestic wood burning was the main source of particulate matter.

With our mobile laboratory we could show that along the Gotthard and San Bernardino route the particulate matter concentrations were much higher in the villages than on the highway. Results of the measurements in Zurich also suggest that wood burning is similarly or even more important. Through active communication of these results we helped to broaden the discussion, and low-tech wood burning such as fire places in the living room, finally got a similar amount of attention as traffic.

Are diesel traffic and wood burning the main sources of particulate matter?

In Zurich and on the Swiss Plateau, the combined contribution of particulate traffic and wood burning emissions is less than 25%. Most particulate matter is formed by oxidation of gases, such as nitrogen oxides, sulphur dioxide, or volatile organic compounds. Traffic contributes more to particulate matter by nitrogen oxide emissions than by direct soot emissions. Soot does not contribute so much in mass but is a highly toxic and carcinogenic substance. To solve the air quality problems, separate strategies are needed to tackle the soot emissions and to reduce the particulate matter concentrations. The LAC is committed to further investigate the complex basics of the air quality but also to communicate the results so that the right decisions can be made to improve our air quality most efficiently.



Figure 1: The PSI mobile laboratory in the Mesolcina valley.

Equipment for the study of diffusion in compacted clay materials

Martin A. Glaus, Luc R. Van Loon, *Laboratory for Waste Management (LES), PSI*

Molecular diffusion is the primary mechanism for the transport of pollutants in the pore water of compacted clay materials. Laboratory scale diffusion experiments are being carried out at LES in order to provide relevant transport parameters and to strengthen the process-based understanding of diffusion in the context of safe geological disposal of radioactive wastes. Specific equipment is needed to confine the compacted clay samples at the desired geometry and to keep them at relevant in-situ pressures. The present contribution gives an overview of equipment specifically designed for such purposes.

The most frequently applied technique is *through-diffusion*, in which two surfaces of a clay sample are contacted with the circulatory systems of two liquid reservoirs, one of which contains the radiotracer under investigation. The relevant transport parameters are obtained by measuring the tracer flux from the source to the target reservoir. *In-diffusion* is applied to contaminants that strongly interact with the clay leading to a delayed transport. Such compounds will only

penetrate a smaller part of the clay sample. Profile analysis of the tracer distribution in the clay sample yields the desired transport properties of the tracer.

Tailor-made equipment was developed at LES in order to accommodate the specific properties of the clays [1–3]. Important features and requirements are: (i) Clay stones are exposed to in-situ pressures of up to 15 MPa; many clay minerals produce strong swelling pressures. Shortcuts circuits between the liquid loops must be prevented. (ii) Good contact of the circulating fluid with the clay sample. (iii) Ability to be run in a continuous operation mode.

Figure 1 shows a representative type of pressure cell used for the study of through-diffusion parallel to the bedding of the clay. The pressure applied perpendicular to the bedding can be continuously controlled. Variations of this cell type are used to study diffusion perpendicular to the bedding and for swelling clay minerals. Insulation of the inner surfaces with PEEK is applied for additional electrochemical measurements. Techniques to analyse tracer profiles with a resolution at 10 μm scales were developed for clay stones and clay minerals [2,3].

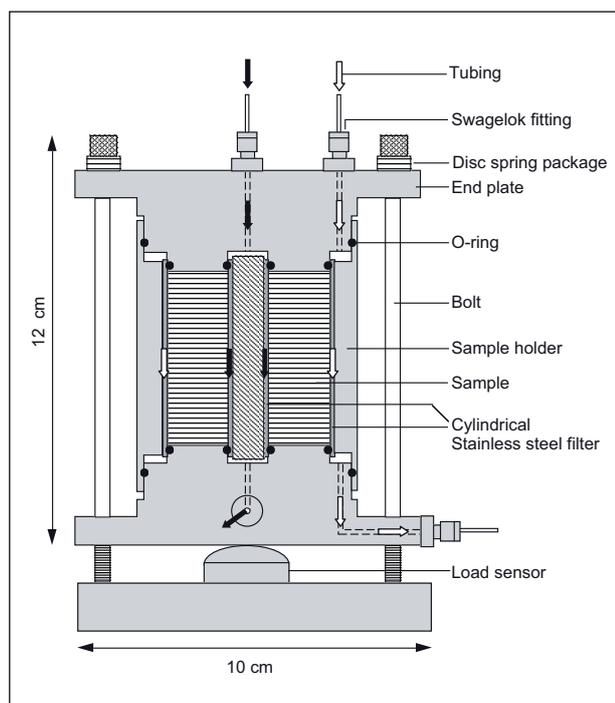
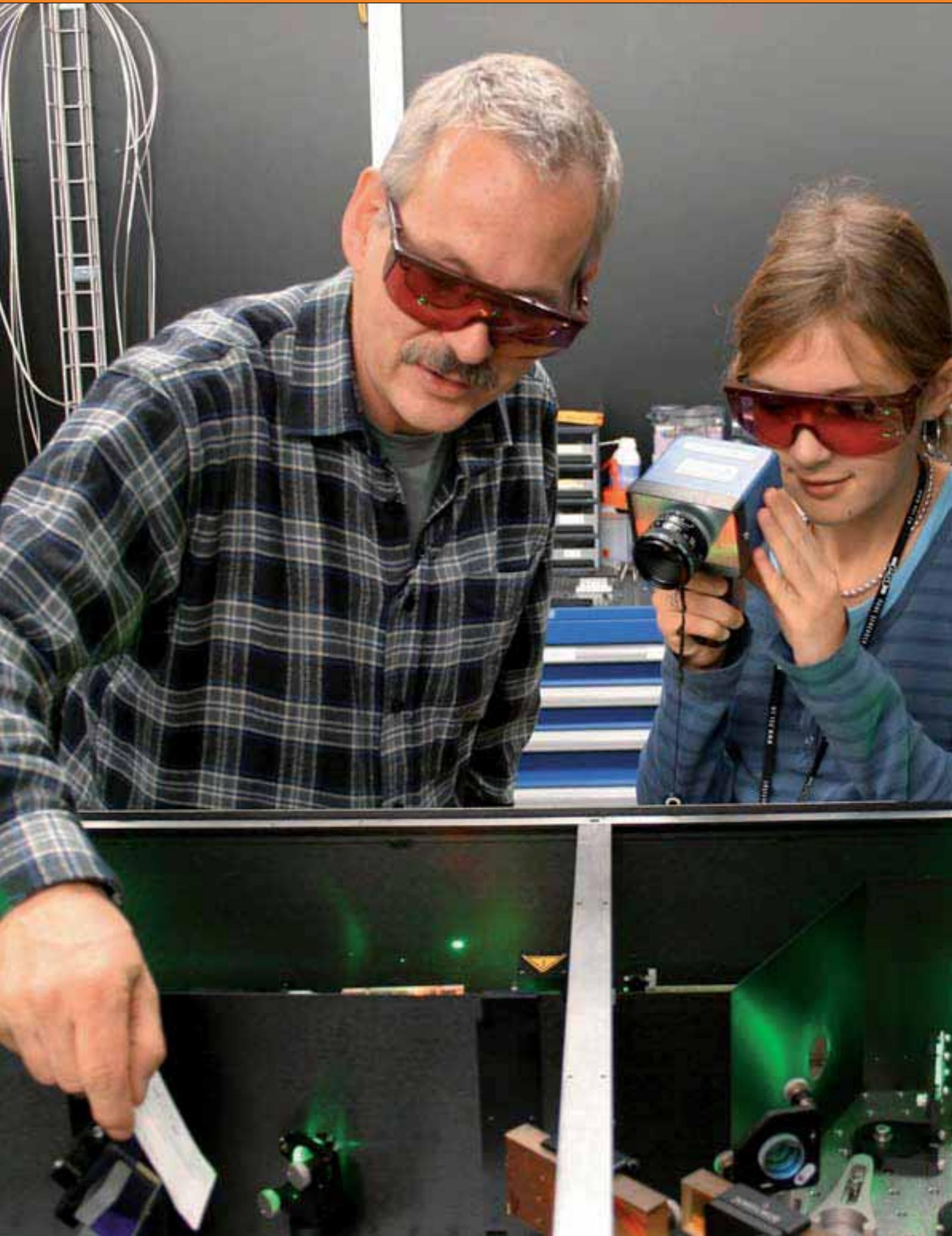


Figure 1: Diffusion cell for the study of diffusion parallel to the bedding of the clay stone (horizontal hatch). Black and white arrows represent the pathways of the circulating fluids of the source and target reservoirs, respectively.

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Research centre and user lab

The Paul Scherrer Institute (PSI) is a multi-disciplinary research centre for natural sciences and technology. Research priorities lie in areas of basic and applied research, particularly in fields that are relevant for sustainable development, as well as of major importance for teaching and training, but which are beyond the capabilities of a single university department. In national and international collaborations with universities, other research institutes and industry, PSI is active in solid-state research, materials sciences, elementary particle physics, life sciences, nuclear and general energy research, and energy-related ecology.

The institute is committed to future generations by paving the way for sustainable development of society and economy. Through its research, PSI acquires new basic knowledge and actively pursues the application of this knowledge within industry.

With 1,270 employees, it is the largest national research institute and is unique in Switzerland. PSI develops and operates complex research installations that call for especially high standards of know-how, experience and professionalism, and is one of the world's leading user laboratories for the international scientific community.

'Bring your daughter to work day' gave physicist Paul Beaud a chance to show his daughter Muriel a laser lab at the SLS.

(Photo: Beat Gerber)

Research and user labs

PSI's total expenditure on R&D, construction and operation of research facilities, infrastructure and services in the year under review amounted to CHF 288.9 million. The Swiss Federal Government provided 80% of this figure, amounting to CHF 230.4 million.

Investments reached CHF 47.4 million (16% of total budget). HR costs comprised CHF 165.5 million (57%). Third party funding rose by some CHF 10 million on the previous year, and Swiss federal funding also rose slightly, with the result that total expenditure – including the contribution to the Energy and Mobility Competence Centre (CEM) – exceeded CHF 290 million.

Third party funding in 2006 amounted to CHF 52.9 million, 60% of which came from private business and 20% from federal Swiss research programs (Swiss National Fund, Federal Ministry of Energy); 15% derived from EU programs.

PSI Financial Statement (in CHF millions)		
	2006	
Expenses		
Operations	241.5	84 %
Investments	47.4	16 %
Total	288.9	100 %
Thereof from:		
Federal government funding	230.4	80 %
Third party expenditure	58.5	20 %
HR (incl. trainees, ongoing staff education and scheduled work)	165.5	57 %
Third party revenue from		
Private industry	25.4	48 %
Federal Research Fund	10.4	20 %
EU programs	8.0	15 %
Other	9.1	17 %
Total	52.9	100 %

70 % to user lab

Some 70% of total expenditure in 2006 was linked to PSI's function as a user laboratory. High pressure from the largely external body of users continued to restrict the time available for the Institute's own research activities. Long-term this

User lab 2006						
	SLS	SINQ*	SpS	Particle physics	PSI Total	(2005)
No. of beamlines/instruments	11	12	6	11	40	(35)
No. of experiments	653	260	135	10	1058	(1141)
No. of user visits	1990	328	130	337	2785	(3025)
No. of users	934	259	95	133	1421	(1432)

* Reduced service due to the MEGAPIE experiment.

tendency should not be encouraged, as PSI can only provide optimal support and consultative services for external users if its own research remains at a constant high level.

At year-end 2006 some 1270 people were employed full-time at PSI. Three-quarters of these (approx. 75%) live in Canton Aargau, some 10% in Canton Zurich, the rest in other cantons and in border areas outside Switzerland. 15% of employees are women (13% of scientific staff), and almost two-fifths of all employees (38%) hold a foreign passport.

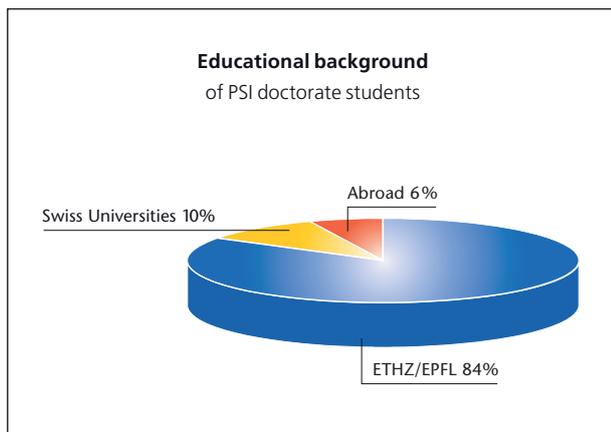
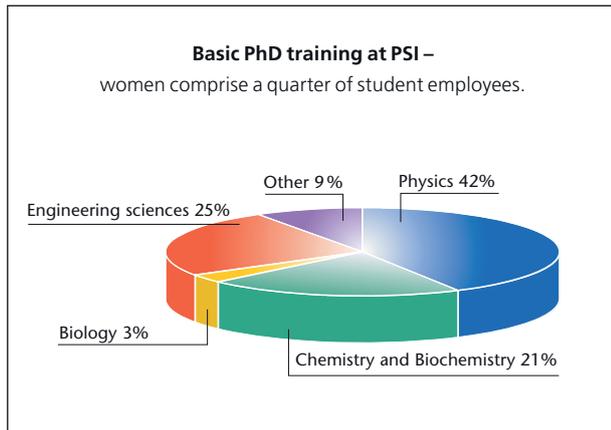
Training facilities in high demand

In the year under review 270 postgraduates completed their PhD theses wholly or partly at PSI, benefiting both from the research facilities and from the support of PSI staff. More than 170 of these were funded by PSI. At year-end 2006 PSI employed 78 apprentices in 12 different training fields.

With its commitment to doctoral education, as well as to teaching at the two Swiss Federal Institutes of Technology (ETH) and at classical and applied sciences universities, PSI is a major source of input to the Swiss Graduate School sector. Recognized the world over, our leading-edge research, as well as our globally networked user lab operations, guarantee that students are trained at internationally competitive levels. More than 70 PSI scientists had teaching commitments at classical and applied science universities in 2006.

Taking the strain off the Swiss universities

In 2006 PSI spent some CHF 30 million on training and infrastructure facilities for PhD students, as well as on university teaching. Some 80% of this outlay was allocated to postgraduates from universities and from the Zurich and Lausanne ETH institutes. By providing research training and lab facilities for postgraduates and external research groups, PSI takes a



considerable financial and academic load off the shoulders of the Swiss universities.

Alongside academic and vocational training, PSI also offers courses on radiation protection and reactor technology. The special schools established for that purpose were attended by more than 2000 professionals in 2006.

Research at PSI is closely linked to the design, development and operation of large, complex research facilities. Unique in Switzerland, we are also, thanks to this specialty, the biggest national scientific research institute. Indications of our success and standing are on the one hand the number of papers published by our scientists in refereed journals, and on the other the impact score that tells how often publications are cited by other researchers.

Bibliometric data supplied by the University of Leiden shows that the output of scientific articles from PSI has again risen in recent years. It now stands at 800 per year as against a ten-year average of approximately 500. The impact score has likewise risen and currently stands at 2500 per year. This means that on average each paper is referred to between three and five times by other scientists.

An attractive cooperation partner

The main focus of this impact score coincides with our principal research fields – solid-state and particle physics, bio-sciences and energy research – demonstrating a close fit between PSI's research profile and scientific output. Some 80% of our publications are in these core areas. Analysis of various collaborations shows that PSI is an attractive partner, above all at the international level. This, as well as the Institute's outstanding impact score, puts us among the world leaders.



SLS

The Swiss Light Source (SLS) is a massive microscope and giant X-ray machine all in one. It accelerates electrons to nearly the speed of light and steers them with special magnets so that the characteris-

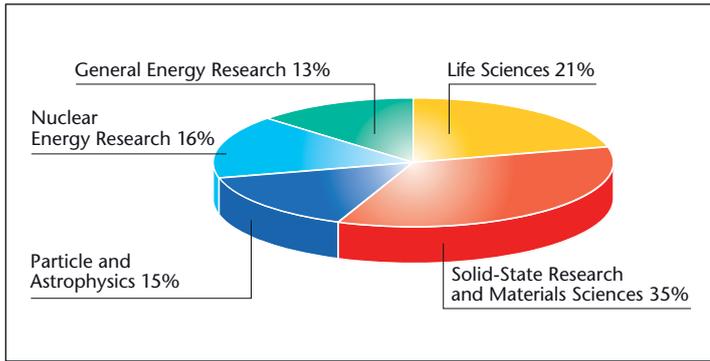
tic high intensity synchrotron light is generated straight ahead. This electromagnetic radiation spanning the wavelengths from infrared to hard X-ray light is ideally suited to structural analysis of matter as well as spectrometry and to the ultra-fine structuring of material surfaces in the nanometer range.



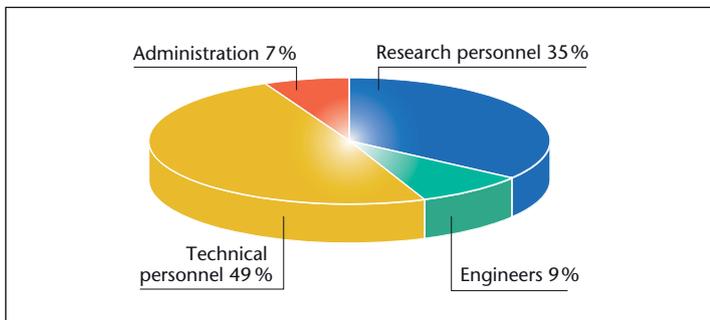
Neutrons for MARS

MARS is the latest instrument at SINQ. Due to its high energy resolution this backscattering spectrometer greatly enlarges the range of experimental possibilities. MARS received

first neutrons in October 2006 and ten days later the first spectrum was created. From summer 2007 onwards the instrument will be available to the users.



In the total budget distribution for 2006 (incl. external funding) across PSI divisions, research facilities – in particular accelerator, SLS and SINQ – were allocated to the various departments.



HR structure clearly reflects PSI's function as a user lab. The large-scale facilities and complex research equipment require a high technical staffing level.

PSI as a user lab

PSI aims to continue attracting the best international scientists in their fields. This means that our employees, our research spectrum and infrastructure as well as our vital research culture must all meet the highest demands.

Nationally as well as internationally, PSI has established itself as a leading user laboratory. In 2006 we had some 3000 visits from more than 1400 scientists who carried out over 1000 experiments. Approximately 40% of lab users are from PSI and the Swiss universities, and more than half are from the EU; in total over 60 different nationalities from 31 different countries. Results of the research from the large facilities; SLS, SINQ, and S μ S resulted in 426 scientific publications (previous year 280), among them a larger number than ever in top journals like Science, Nature, Cell, Langmuir and Physical Review Letters.

The annual expenditure for the development and running of research facilities for the use of the Swiss universities amounts to some 40 Million CHF.

Intense demand for SLS beam time

The Swiss Synchrotron Light Source (SLS) at PSI has been operating for five years. In the year under review 934 researchers conducted 653 experiments with this giant microscope, profiting from the exceptional qualities of a facility that is among the world's best.

Current research projects using the synchrotron's beamlines cover a wide area. They include the investigation of protein structures – crucial for the development of pharmaceuticals as well as for research into the function of the human genome – or the creation of 3-D reconstructions of biosystems, or the



SINQ

The **Spallation Neutron Source (SINQ)** is another oversized microscope. It produces neutrons, which at PSI are mostly used for experiments in materials research, solid-state physics (e.g. superconductors, magnetic and ferroelectric materials) and technology (neutron radiography). The neutrons are produced via spallation reactions induced by bombarding heavy metals (e.g. lead bismuth for MEGAPIE) with a proton beam from the accelerator.

perconductors, magnetic and ferroelectric materials) and technology (neutron radiography). The neutrons are produced via spallation reactions induced by bombarding heavy metals (e.g. lead bismuth for MEGAPIE) with a proton beam from the accelerator.



S μ S

Harnessed to the proton accelerator the **Swiss Muon Source (S μ S)** produces muons by directing the proton beam on a carbon target. When implanted in matter, these unstable elementary particles function like minute gyroscopes, providing precise information about local internal magnetic fields. Thanks to their spins, muons serve as highly sensitive probes used widely in materials and solid-state research.

Thanks to their spins, muons serve as highly sensitive probes used widely in materials and solid-state research.

investigation of structures and properties of new materials and material surfaces.

The high stability of the SLS beamlines has resulted in intense demand for user time, and we are stepping up our provision to meet this as rapidly as possible. Eleven beamlines were in use at the SLS in 2006, and a further eight were in various stages of planning, construction and commissioning.

Proton accelerator in demand on all fronts

The proton accelerator was originally developed more than 30 years ago for research into the basic physics of elementary particles. Today it is mostly used to produce neutrons in the Spallation Neutron Source (SINQ), the most powerful of its kind in the world. The facility comprises twelve instruments for neutron experiments, used in 2006 by around 260 scientists from Switzerland and other countries. This was an outstanding year for SINQ with the operation phase of the MEGAPIE liquid metal target being completed (p. 104).

Central to SINQ research are solid-state physics and materials sciences. Significant for future applications are high-temperature superconductors (HTS), which at certain temperatures can conduct electricity without losses. At the moment the upper temperature limit is minus 135 degrees Celsius. In order to make further progress the origins of HTS have to be understood; a challenge for the researchers at SINQ. A speciality of SINQ is the further examination of materials which combine electrical and magnetic properties. This is usefully applied to the development of materials used in sensors, transducers and the performance of computer hard drives.

A third of the proton beam is used for producing the world's most intensive continuous muons, which are used as probes for structural research in materials sciences, solid-state physics and

chemistry. Six instruments are currently available for this research. In 2006 they were used by 95 scientists in 135 projects.

Unique research offer

PSI's three major experimental research facilities, SLS, SINQ and S μ S, offer an internationally unique combination of complementary methods for structural research, spectroscopy and materials structuring. The EU's Large Scale Facility Access programme supports this provision with funding to PSI of around CHF 1 million per year, which is used for operating the beamlines, ongoing development of the equipment, and training and support of researchers from EU countries working on these major facilities.

As the demand for laboratory places and instruments is up to five times what PSI can supply, only top research projects can be allotted time on the beamlines. Allocation is based on research proposals assessed for merit by an international board of scientific experts.

Active in environmental research

Research into environmental situations and the development of environmentally friendly technologies frequently demands complex facilities and equipment. PSI operates and develops large scale facilities that are in continuous intensive use in these sectors. For example, two SLS beamlines will soon be used for studying the mechanisms of dispersion and intensification of environmental pollutants, as well as questions relating to the long-term disposal of nuclear waste. The proton accelerators enable production of short-lived radio-nuclides for use in atmospheric chemistry experiments.



Particle physics

Particle physics investigates the fundamental building blocks of matter and their interactions. Many experiments have confirmed the standard physical model with great exactitude, but one element of this theoretical structure – the Higgs boson – has not yet been found. Particle physics is currently engaged on a twofold quest, on the one hand for this heavy particle and on the other for a new super-symmetry that will link elementary particles and their interactive forces, including gravity.

ment of this theoretical structure – the Higgs boson – has not yet been found. Particle physics is currently engaged on a twofold quest, on the one hand for this heavy particle and on the other for a new super-symmetry that will link elementary particles and their interactive forces, including gravity.



The hot-lab

The PSI hot-lab is home to applied materials research on highly radioactive probes and radioactive waste disposal. The only facility of its type in Switzerland, it provides backup for Swiss nuclear power plants as well as for university and industrial research groups.

power plants as well as for university and industrial research groups.

The SINQ facility is used for neutron radiography investigating the distribution of liquids and gases in fuel cells in order to establish fundamental processes for efficient energy conversion. Processes for the production of solar hydrogen as an environmentally friendly alternative to fossil fuels are undergoing further development in PSI's solar furnace.

A new accelerator-based mass spectrometer that enables radio-carbon dating (using the C₁₄ method) of very small samples is being used in climate research for analyzing ice cores. And in the PSI smog chamber scientists are simulating the formation of aerosols in order to investigate the behaviour of these climatically relevant suspension particles in air.

Top quality for atomic particle physicists

PSI's proton beam also functions as an intensive secondary source of pions and muons, which are used for experiments in particle physics. Because of their exceptional quality – they are the world's best – they are highly sought after by American and Japanese as well as European scientists. Researchers are currently investigating the basic properties of pions and muons, looking in particular at subtle details that are crucially important for present-day particle physics. Data from experiments successfully completed by scientific teams from Europe, Russia and the USA are currently being evaluated and results will be available in 2007.

Important news from particle physics at PSI is the development of extremely sensitive detectors, used for example in the CMS experiment at CERN, which should prove the existence of heavy particles; as predicted by the standard model of physics. Production of pixel detectors for CERN was stepped up in 2006 in order for them to be built into the CMS in 2008.

Tissue-sparing cancer therapy

The PROSCAN project for extending proton therapy to deep-seated tumours has seen major progress in 2006. COMET, the new superconductive compact cyclotron, came into operation and after successful testing with the current treatment facility, Gantry 1, came on stream for patient treatment in early 2007.

PSI has granted industrial licenses for its precision radio-therapy scanning technology. A privately financed commercial facility in Germany using the scanning process and compact cyclotron developed at PSI will soon commence operations. Further projects are in planning or construction phase. With contracts in the double figure range (CHF millions) for the delivery of components and systems; Swiss industry stands to gain from this unique PSI-developed technology.

A new treatment gantry - Gantry 2 is under construction and will be ready to treat patients towards the end of 2008. This facility will have the ability to treat moving tumours, such as in the chest.

From 2009, there will then be two highly precise radiation facilities for proton therapy dedicated to patient treatment (no research) with the capacity to treat 500 – 600 patients a year. There will also be a new eye tumour treatment facility (OPTIS 2) coming into operation at the end of 2007. In 2006 more than 200 patients were successfully treated in the current OPTIS.

Project Manager Roland Horisberger stands in the giant CMS detector at CERN where PSI's detector chips will be installed.

(Photo: H.R. Bramaz)



The solar furnace

PSI's solar concentrator, an 8.5 m diameter concave mirror, bundles solar radiation to an intensity of 5000 suns. The high temperatures (up to 2000° C) created in a reactor aperture are used for re-

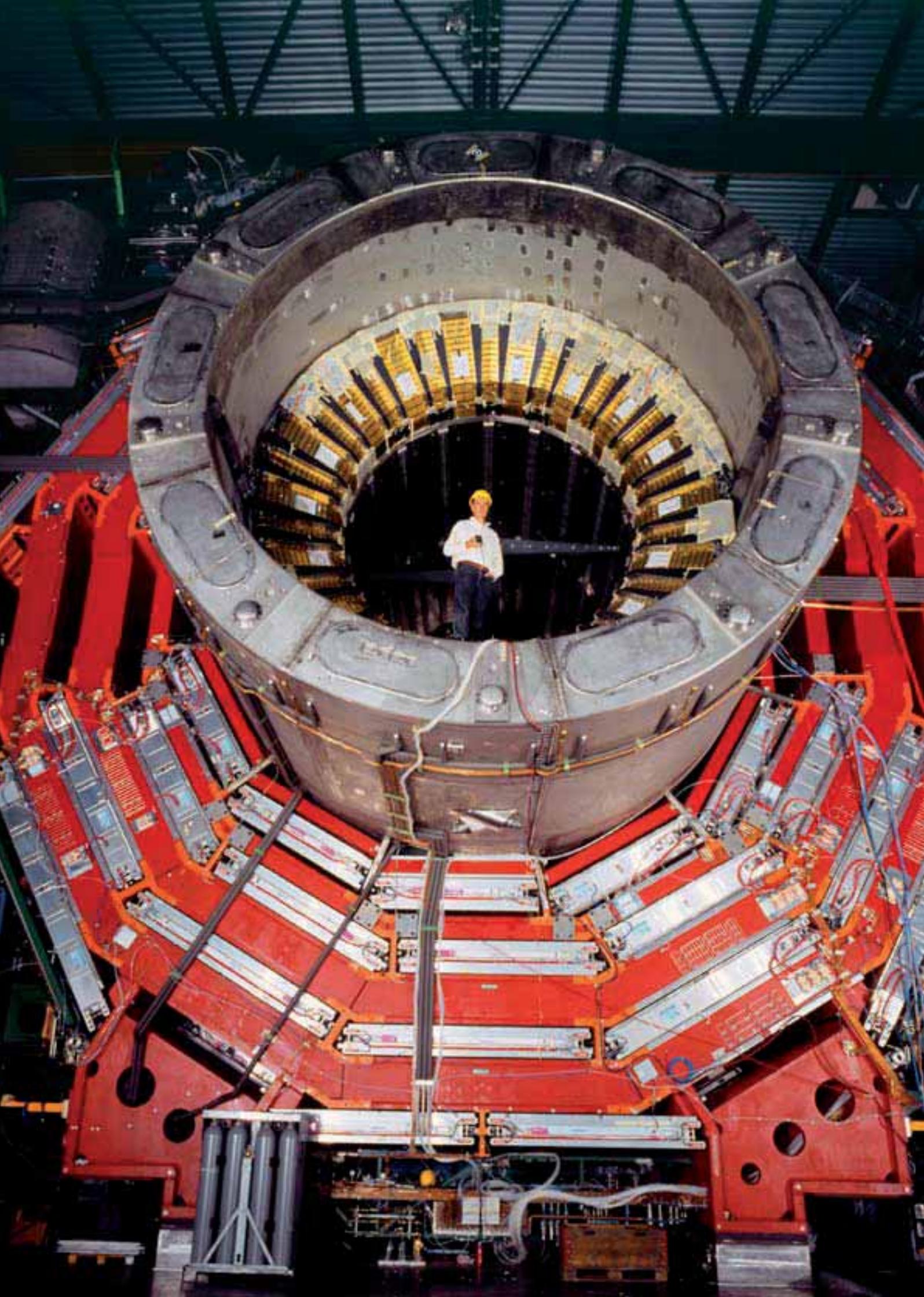
search into solar-chemical processes such as the efficient production of solar fuels and innovative materials. A high-flux solar simulator of double this power was recently installed for experiments into radiation under controlled conditions independent of the weather.



The smog chamber

The smog chamber simulates conditions for experiments in atmospheric chemistry. A 27 m³ Teflon sack can be filled, for example, with exhaust gases for exposure to artificial sunlight, and the ensuing chemical reactions can be observed and measured.

Results can be used, for example, to determine how particulate matter transforms in the atmosphere.



Commission and committees

(status end of 2006)

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Super heavy machinery for proton therapy (Gantry 2) is carefully positioned.

(Photo: Beat Gerber)

LIST OF PUBLICATIONS

Synchrotron Radiation and Nanotechnology (SYN)

UNIVERSITY LEVEL AND OTHER TEACHING

J. Gobrecht

Nanotechnologie für Ingenieure

Fachhochschule Nordwestschweiz, Windisch, SS 2006

Halbleiter-Laser

2 Lektionen im Rahmen des Weiterbildungskurses „Laserbearbeitungstechnik“ der ETHZ/FHNW, Zürich 2.12.2006

D. Grützmacher u.a.

University Konstanz, SS06

L.J. Heyderman

Magnetic Imaging Techniques

Seminar in Lecture Series “Magnetism and Spin Dependent Transport” (Prof. Rüdiger), Universität Konstanz, Germany, 10.7.2006

T.A. Jung

Blockkurse Nanowissenschaften 12 KP

Studiengang Bachelor in Naturwissenschaften mit Vertiefungsrichtung Nanowissenschaften, WS06/07

T.A. Jung u.a.

University Basel

J. Lobo

Teaching assistant in the Physic's laboratories for second year Biology students

1st semester University Zurich, WS06/07

E. Müller

Electron Microscopy

ETH Zürich, SS06

E. Müller u.a.

Electron Microscopy

ETH Zürich, WS06/07

F. Nolting

Photo-Elektronen Mikroskopie

Gastvorlesung in: Physik auf der Nanometerskala II, H.W. Fink, University Zurich, 2.2.2006

B. Patterson, Th. Greber

University Zurich

H. Schiff

Nanotechnologie für Ingenieure

Fachhochschule Nordwestschweiz, Windisch

SS 2006

LIGA technology

Seminar for Master of Micro- and Nanotechnology (MNT), Buchs, Switzerland, 23.2.2006

PANAMA Summer School on Emerging Nanopatterning Methods (EU Project NaPa)

- *Social and ethical implications of nanotechnology*

- *Panorama of nanopatterning methods*

- *Nanoimprint lithography*

Toulouse, France, 3.-14.7.2006

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Master of Engineering in Packaging Technology, International Packaging Institute (IPI),

Neuhausen, Switzerland, 26.10.2006

H. Sehr

Embedded MEMS Lab: Layer Deposition

Eidgenössische Technische Hochschule Zürich, Switzerland, 5.7.2006

H. Sigg

Synchrotron-Halbleiter-Praktikum

University of Zurich, SS 2006

J.F. van der Veen

Bachelorstudiengang Informatik

ETH Zürich, SS06 Physik

Materials Research using Synchrotron Radiation

ETH Zürich, WS06/07

H.J. Weyer

University Basel, WS06/07

Ph. Willmott

University Zurich

ETH Zurich, WS06/07

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F. Nolting, (Ch. Schönenberger, University Basel)
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Lausanne Switzerland, 14.2.2006

M. Janousch
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Paul Scherrer Institut, Villigen, Switzerland, 20.-21.2.2006

T.A. Jung
Workshop on Nanoanalysis
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C. Schulze-Briese
The full spectrum - Biology between IR and Hard-Xrays - and beyond
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M. Stampanoni
Parallel session 'Tomography'
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PUBLIC RELATIONS

J. Gobrecht

- Presentation of SLS Micro-Tomography beamline and start-up company EULITHA GmbH at Hannover Fair, Hannover, Germany, 15.-18.4.2006
- Representation (Booth) of institute INKA at Nano-Europe fair, St. Gallen, Switzerland, 12.-14.9.2006
- Representation (Booth) of institute INKA at “Fachmesse Kunststoffmaschinen (FAKUMA)”, Friedrichshafen, Germany, 20.-21.9.2006

T.A. Jung

- *Nano-Wissenschaft ...und der Bedarf nach Normierungen*, Schweizerischer Normenverband, Workshop ‘Nanotechnologie und Normierungen’, Winterthur, Switzerland, 26.4.2006
- *Presentation and Panel Discussion on Nanotechnology*, ‘Schlossgespräche’, Schloss Überstorf, Überstorf (Switzerland), 17.11.2006

P. Morf

- Conference Report on the “1st International Workshop on 'Electrical Functionality in Nanoarchitectures'”, Small, 4, 4 (2006)

F. Pfeiffer

- *Bessere Röntgenbilder in der Medizin durch Phasenkontrast*, Vortrag am PSI Contact Evening, 27.10.2006

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DISSERTATIONS

D. Grützmacher

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G. Palfinger, University of Konstanz (2006)

T.A. Jung

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M. Wahl, University of Basel, Switzerland, (2006)

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A. Kiebele, University of Basel, Switzerland, (2006)

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Electronic transport, field effect and doping in pentacene nanorods and monolayer thin film prepared by combination of nano-fabrication and self-assembly

C. Vanoni, University of Basel (2006)

H. Sigg, V. Schlott

Single-Shot Electron Bunch-Length Measurements with a spatial electro-optical-auto-correlation interferometer using coherent Transition radiation at the 100 MEV SLS pre-injector LINAC

D. Sütterlin, Diss. ETH No. 16668 (2006)

J.F. van der Veen

X-Ray Scattering Studies of Complex Liquids in Nanometer-Sized Containers

H. Keymeulen, ETH Zürich, Switzerland, February 2006

X-Ray Scattering Studies of Ordering Phenomena in Colloids Confined in Microcavity Arrays

A. Díaz, ETH Zürich, Switzerland, October 2006

AWARDS

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3 dimensional Ge quantum dot crystals prepared by templated selforganization

Best Poster Award, 2006 Advanced Research Workshop, Future Trends in Microelectronics, Crete, Greece, 26.-30.6.2006

MEMBERSHIPS IN EXTERNAL COMMITTEES

R. Abela

- Chairman of the Scientific Advisory Committee ESRF (France)
- Chairman of the Scientific Advisory Committee ALBA (Spain)
- Chairman of the Swiss-Norwegian Foundation for Research with X-Rays
- Member of the Scientific Advisory Committee of DIAMOND (UK)

C. David

- Member of the International Program Committee of the Micro- and Nano-Engineering Conference 2006
- Member of the International Consortium for Coherent X-ray Diffractive Imaging (ICCDXI)
- Member of the ESRF Beamline Review Panel of ID01
- Member of the ESRF Beamline Review Panel of ID19

J. Gobrecht

- Vice director "Technology" and head of module "Applied projects", Swiss Nanoscience Institute, University of Basel, Switzerland
- Board member, Swiss Micro- and Nanotechnology Network (CTI/KTI)
- Member of team, ETH Competence Center Materials Science (CCMX), ERU "Materials for life sciences"
- Scientific advisory committee of network "Nanocluster Bodensee", Switzerland
- Member of thesis advisory committee for PhD candidate Ch. Weiteneder, University of Neuchatel, Switzerland
- Member of review committee for the Central Microstructures Facility of Rutherford Appleton Laboratory, Great Britain

T.A. Jung

- Technikverständnis in der Allgemeinbildung' Kommission der wissenschaftlichen Akademien Schweiz
- Scientific Board of the NCCR Nanoscience, Co-chair of the module 'Molecular Electronics'
- Editorial Board Member, Europhysics News
- Scientific Committee for Newly Identified and Emerging Health Risks, (SCENIHR) Health and Consumer Protection Directorate Gener Scientific Committee advising the European Commission

F. Nolting

- Program Committee, International Workshop on Nanoscale Spectroscopy and Nanotechnology, NanoSS4
- Member of Proposal Review Committee Soleil, France

C. Quitmann

- Member Advisory Committee Nanoscience beamline at DIAMOND, UK
- Member of the Editorial board (Surface, Interface and Atomic-Scale Science) Journal of Physics: Condensed Matter
- Member of the board of the Center of Excellence in Analytical Chemistry

H. Schiff

- AVS American Vacuum Society, NSTD Nanometer-scale Science and Technology Division, elected board and executive committee member
- MNC Micro- and Nanoengineering conference (Japan), International Program Committee
- NNT Nanoprint and Nanoimprint conference, committee member

C. Schulze-Briese

- ESRF Methods and Instrumentation Proposal Review Committee
- ESRF MX-beamline review panel
- Australian Synchrotron PX-beamline advisory panel

H. Sigg

- Advisory Committee, International Conference on Intersubband transition in quantum wells

J.F. van der Veen

- Science Advisory Committee of Elettra, Trieste
- Scientific Committee for Inorganic and Analytical Chemistry, Science Foundation, Flanders, Belgium
- Chairman of Programme Committee of PSI Summer School on Condensed Matter Research, Zuoz, Switzerland
- Scientific Advisory Committee of HERCULES, Grenoble
- Science Advisory Committee of the Advanced Light Source, Berkeley, USA
- International Advisory Committee of the International Conference Series on Synchrotron Radiation Instrumentation
- Science Advisory Committee of Synchrotron SOLEIL, Gif-sur-Yvette, France
- Advisory Committee of the International Conference Series on Surface X-Ray and Neutron Scattering
- Member Steering Committee CCMX, Competence Centre for Materials Science and Technology
- Member Steering Group NCCBI, National Competence Center in Biomedical Imaging

H.J. Weyer

- Correspondent, Synchrotron Radiation News

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UNIVERSITY LEVEL AND OTHER TEACHING

S. Adam

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University of Applied Science Zürich, Switzerland, WS 2005/06, SS 2006

A. Adelman

Statistics and Probability Theory

University of Applied Science Zurich, Switzerland, WS 2006/07

J. Jourdan, B. Krusche, D. Rohe

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University of Basel, Switzerland, WS 2006/07

L. Rivkin

Introduction to Particle Accelerators

EPFL, Lausanne, Switzerland, WS 2006/07

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ICTP School on Synchrotron Radiation and Applications, Trieste, Italy, May 2006

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Spectroscopy/Microscopy, 5th PSI Summer School on Condensed Matter Research, Zuoz, Switzerland, August 19-26, 2006

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Synchrotron Radiation and Dynamics with Radiation

CERN Accelerator School, Zakopane, Poland, October 2-14, 2006

M. Schneider

Grundlagen der Elektronik

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U.D. Straumann, U. Langenegger, M. Dittmar, K. Müller, O. Steinkamp, A. Streun

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A. Anghel, P. Bruzzone, M. Vogel

Results of Contact Resistance Distribution in ITER-Size Conductor Termination
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H.P. Bijl, P. van Luijk, R.P. Coppes, J.M. Schippers, A.W.T. Konings, A.J. van der Kogel

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W. Roser

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A. Adelman

Dynamics of High Intensity Beams in Cyclotrons
TRIUMF Cyclotron Division, Vancouver, Canada, May 19, 2006

A. Adelman

High Intensity Cyclotron Simulations: Towards Quantitative Predictions
ICFA-HB2006, KEK, Tsukuba, Japan, May 29 - June 2, 2006

A. Adelman

Scalable Algorithms and Applications in Particle Accelerator Modeling
ISC 2006, Dresden, Germany, June 27-30, 2006

M. Böge

SLS Status Report
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M. Böge

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86th Eastern Forum of Science and Technology Shanghai, China, December 7, 2006

M. Böge

CORBA based Beam Dynamics Applications at the SLS
SSRF, Shanghai, China, December 11, 2006

M. Dehler

Resonant strip line design for the European XFEL intra bunch train feedback
Workshop on Longitudinal Beam Stability in Linear Accelerators, Schloss Böttstein, Böttstein, Switzerland, March 8-9, 2006

M. Humbel

Commissioning of a 50/150 MHz Buncher Combination in the 870 keV Injection Line of PSI Injector 2
XXXV ECPM, Nice, France, November 2-4, 2006

W. Joho

The SLS facilities
Brookhaven National Light Source, Brookhaven, USA, August 2, 2006

B. Keil

Digital System Concept for the Intra Bunchtrain Feedback for the European X-FEL
Workshop on Longitudinal Beam Stability in Linear Accelerators, Schloss Böttstein, Böttstein, Switzerland, March 8-9, 2006

B. Keil

An Intra Bunch Train Feedback System for the European X-FEL
FLS 2006, Hamburg, Germany, May 18, 2006

Ch. Kraus

Comparison of h- and p- Refinement in a Finite Element Maxwell Time Domain Solver
9th ICAP, Chamonix Mont-Blanc, France, October 2-6, 2006

V. Schlott

Evolution of Free Electron Lasers – from IR to X-Rays
Fakultätskolloquium, Universität Leipzig, Germany, October 6, 2006

J.M. Schippers

PSI-Experience with the new cyclotron for PSI's proton therapy facility PROSCAN
Seminar, Centre de Protonthérapie d'Orsay, Orsay, France, February 20, 2006

J.M. Schippers

Overview of PSI's proton therapy program and PSI's new facility PROSCAN
Seminar, Erasmus University Medical Center, Daniel den Hoed Kliniek, Rotterdam, The Netherlands, April 18, 2006

J.M. Schippers

The SC 250 MeV cyclotron and beam lines of PSI's new protontherapy facility PROSCAN
Int. Conference on Applications of Accelerators in Research and Industry (ICAARI), Fort Worth, USA, August 20, 2006

J.M. Schippers

Instrumentation development for proton therapy
Seminar, Paul Scherrer Institut, Villigen, Switzerland, August 30, 2006

J.M. Schippers

The SC cyclotron and beam lines of PSI's new protontherapy facility PROSCAN
Europ. Cyclotron Progress Meeting (ECPM) 2006, Nice, France, November 2-4, 2006

P.A. Schmelzbach

1.8 MW Upgrade of the PSI Accelerator Facility
iThembaLABS, Faure, South Africa, March 14, 2006

P.A. Schmelzbach

Operation of the PSI Megawatt Accelerator Facility
iThembaLABS, Faure, South Africa, March 16, 2006

P.A. Schmelzbach

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ICFA-HB2006, KEK, Tsukuba, Japan, May 29 - June 2, 2006

P.A. Schmelzbach

1.8 MW upgrade of the PSI proton facility
EPAC 2006, Edinburgh, UK, June 26-30, 2006

M. Schneider

Coaxial Switch, High Power Load and Higher Harmonic Absorber for PROSCAN
Fourth CW and High Average Power RF Workshop, Argonne National Laboratory, Argonne, Illinois, USA, May 1-4, 2006

A. Strinning

Decommissioning of the MEGAPIE Target
Int. Workshop on Heavy Liquid Metal Spallation Targets for Transmutation, Aix-en-Provence, France, November 30, 2006

F. Stulle

Options for the second Bunch Compressor Chicane of the CLIC Main Beam Line
CLIC ILPS Meeting, CERN, Geneva, Switzerland, February 7, 2006

F. Stulle

Status of the CLIC Bunch Compressor Work at PSI
CLIC Meeting, CERN, Geneva, Switzerland, October 6, 2006

S. Teichmann

Shielding parameters of concrete and polyethylene for the PSI proton accelerator facilities
8th Workshop on Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF 8),
Pohang Accelerator Laboratory, Republic of Korea, May 22-24, 2006.

D. Treyer

RF Front Ends for Transversal BPM
Workshop on Longitudinal Beam Stability in Linear Accelerators, Schloss Böttstein, Böttstein,
Switzerland, March 8-9, 2006

W. Tron

Modern and Crowbarless HVPS
Fourth CW and High Average Power RF Workshop, Argonne National Laboratory, Argonne,
Illinois, USA, May 1-4, 2006

M.J. van Goethem

Conceptual design of a nozzle for OPTIS2
44th Workshop of the Proton Therapy CoOperative Group, Zürich, Switzerland, June 16-18, 2006

WORKSHOPS

A. Adelman

Co- Organizer
Workshop on High-Performance Computing
ETH Zurich, Switzerland, September 4-5, 2006

V. Schlott

Organizer
Workshop on Longitudinal Beam Stability in Linear Accelerators
Schloss Böttstein, Böttstein, Switzerland, March 8-9, 2006

DISSERTATIONS

S.C. Leemann

*Characterization of Electron Bunches from Field Emitter Array Cathodes for Use in Next-
Generation X-Ray Free Electron Lasers*

Thesis No. 3724, EPFL Lausanne, Switzerland, 2006
Thesis advisors: Prof. Dr. A.F. Wrulich (EPFL/PSI)
Dr. A. Streun (PSI)

D. Sütterlin

*Single-Shot Electron Bunch-Length Measurements with a Spatial Electro-Optical-Auto-Correlation
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Theses No. 16668, ETH Zürich, Switzerland, 2006
Theses advisors: Prof. H. Jäckel (ETHZ)
Dr. H.C. Sigg (PSI)
Dr. V. Schlott (PSI)

MEMBERSHIPS IN EXTERNAL COMMITTEES

A. Adelman

- CSCS "Horizon Project" Steering Committee
- Expert for Mathematics "Maturitäts Exams"
- Int. Super Computing Conference (ISC), Program Committee
- Member of the Project Group "Swiss National Strategic Plan for High Performance Computing and Networking".

M. Böge

- Review of NSLS II - Lattice and Accelerator Configuration, Committee Member

L. Rivkin

- CERN Accelerator School, Advisory Committee
- DESY, Machine Advisory Committee, Germany
- European Physical Society, Accelerators Group Board, EPAC'06 Organizing Committee
- Joint Universities Accelerator School, Program Committee
- PAC 2007 Program Committee
- SOLEIL, Machine Advisory Committee (Chairman)
- Stanford Synchrotron Radiation Laboratory, Scientific Advisory Committee
- International Linear Collider Machine Advisory Committee

W. Roser

- Swiss Society for Radiation Biology and Medical Physics, Board Member
- Comité Electrotechnique Suisse (CES), Member of TC 62

Th. Schietinger

- European Committee for Future Accelerators (ECFA), Member

V. Schlott

- DIPAC 2007, Scientific Programme Committee
- ALBA Spanish Light Source, Machine Advisory Committee
- DIAMOND Light Source, Technical Advisory Committee
- EuroFEL Advisory Board (Chairman)
- In-Kind Review Committee for the European XFEL (Chairman)
- Working Group on Scientific and Technical Issues for the European XFEL (XFEL-STI)
- CARE Governing Board

P.A. Schmelzbach

- Int. Conferences on Cyclotrons and their Applications: Int. Organizing Committee + Program Committee
- Europ. Cyclotron Progress Meetings, Scientific Committee
- OECD/NEA Int. Workshop on the Utilisation and Reliability of High Power Proton Accelerators, Int. Scientific Advisor

D. Vermeulen

- Int. Conference on Accelerator and Large Experimental Physics Controls Systems, Scientific Advisory Committee

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UNIVERSITY LEVEL AND OTHER TEACHING

A.F. Wrulich
Introduction to Particle Accelerator Physics
EPFL, Lausanne, Switzerland, WS 2004/2005

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High Performance Particle Accelerators
EPFL, Lausanne, Switzerland, SS 2005

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R. Ganter

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Thesis No. 3724, EPFL Lausanne, Switzerland, 2006

Thesis advisors: Prof. Dr. A.F. Wrulich (EPFL/PSI)
Dr. A. Streun (PSI)

MEMBERSHIPS IN EXTERNAL COMMITTEES

R.J. Bakker

- Evaluation of the European XFEL TDR, Hamburg, Germany
- EPAC 2008, Organizing Committee
- FEL 2006, Program Committee

A. Wrulich

- CCLRC, UK, Accelerator Science and Technology Advisory Board
- CNAO, I, Comitato Tecnico
- DESY, D, Machine Advisory Committee
- DIAMOND, UK, Technical Advisory Committee, Chair
- ELETTRA, I, Machine Advisory Committee, Chair
- ISAC, AUS, Int. Science Advisory Committee
- NSLS-II, US, Project Advisory Committee
- SESAME, Jordan, Technical Advisory Committee, Chair
- ESFRI, EU, Expert Committee for Hard X-Ray Sources
- EPAC06, Organizing Committee
- Co-Editor of 'Journal of Synchrotron Radiation'

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- A. Aguadero, M.J. Escudero, M. Pérez, J.A. Alonso, V. Pomjakushin and L. Daza
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P. Allenspach

Involvement of Industry in the Developments of MaNEP

MaNEP-meeting, Neuchatel, Switzerland, February 16, 2006

P. Allenspach

Wide Angle Polarizing Analyzer Concepts

PINS Brookhaven, USA, April 6-7, 2006

P. Allenspach

Continuous and Pulsed Neutron Sources

International Summer School Neutron Techniques in Molecular Magnets Jaca, Spain, September 6, 2006

P. Allenspach

Spectrometers at a Pulsed Neutron Source

Workshop on Instrumentation on a Long Pulse Target Station Rencurel, France, September 11-15, 2006

P. Allenspach

Novel Neutron Optics Based on Supermirrors

WINS Berlin, Germany, September 29 – October 1, 2006

A. Amato

Bulk μ SR News

μ SR User Meeting BVRA 2006,

January 25-26, 2006, Paul Scherrer Institute, Villigen, Switzerland.

A. Amato,

Studies of heavy-fermion superconductors by μ SR technique,

ICM2006 satellite conference "Advances in Neutron, Synchrotron Radiation, μ SR and NMR Researches",

August 28-30, 2006, Tokai, Japan

A. Amato,

μ SR study of heavy fermion superconductors,

First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,

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High-Pressure μ SR at PSI,

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September 28-30, 2006, Tsukuba, Japan

D. Andreica

Pressure-induced magnetic ordering in PrCu₂,

High-Pressure PSI Workshop " μ SR Techniques and Applications",

January 25, 2006, Villigen PSI, Switzerland

D. Andreica
 μ SR under pressure: selected results,
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Erik Bitzek
WW1 Seminar, Universität Erlangen-Nürnberg, November 30, 2006 (Invited seminar)

J. Chang, J. Mesot et al.
Interplay Between High- and Low-Energy Excitations in LSCO
5th International Conference Stripes 2006, Roma, Italy, December 17-19, 2006

K. Clausen
PSI research facilities – and their planned development
First Swiss Japan Workshop on the application and on new development in muon spectroscopy and novel materials
Tsukuba Japan, 28 – 30 September 2006

K. Conder
Layered perovskite cobaltites
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K. Conder, A. Podlesnyak, E. Pomjakushina, M. Stingaciu
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P. Derlet
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August 1-3, 2006

A. Dönni, H. Kitazawa, L. Keller
Magnetic Neutron Scattering: Experiment and Data Analysis
Neutron Scattering Seminar at NIMS, Tsukuba, Japan, December 21, 2006

D.G. Eshchenko,
Dilute magnetic semiconductors (LE and bulk μ SR),
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U. Filges, G. Zsigmond, J. Saroun
FOCUS intercomparison using VITESS/McStas/Restrax
International Workshop on Applications of Advanced Monte Carlo Simulations in Neutron
Scattering, Villigen PSI, October 3-4, 2006

U. Filges, P. Allenspach
Instrument simulations and polarized neutrons
PINS workshop, Brookhaven, USA, April 5-7, 2006

A. Furrer
Barocaloric Cooling: A precursor and spin-off of the Discovery of High-Temperature Superconductivity
International Symposium in Honor of J.G. Bednorz and K.A. Müller, Zurich, Switzerland, March
27-30, 2006

A. Furrer

Excitement with Excitations

Kolloquium für Prof. Hans U. Güdel, Bern, Switzerland, July 7, 2006

U. Gasser, C. Eisenmann, P. Keim, G. Maret, H.-H. von Grünberg

Pair Interaction of Dislocations in Two-Dimensional Crystals

Physics of colloidal dispersions in external fields, Bonn, Germany, March 20-22, 2006

T. Geue, T. Gutberlet, J. Kohlbrecher, J. Stahn

SANS and neutron reflectometry as tools to characterize hard and soft condensed matter nanomaterials

Workshop Nanospectroscopy using Synchrotron Radiation, PSI, Villigen, Switzerland, July 12-14, 2006

H. Grimmer

Black-white symmetry, ordered magnetics, anisotropy of magnetic properties

Satellite Conference on Mathematical and Theoretical Crystallography of the XXIII European Crystallographic Meeting (ECM-23) Leuven, Belgium, August 4-6, 2006

T. Gutberlet

Solid-Liquid Interfaces and their Interaction with Biomembranes

Seminar Graduiertenkolleg „Struktur Dynamik Beziehungen in mikrostrukturierten Systemen“, Uni Dortmund, Germany, February 10, 2006

T. Gutberlet

Ideas about reflectometry with VCN

Workshop on Present Status and Future of Very Cold Neutron Applications, PSI, Villigen, Switzerland, February 13-14, 2006

T. Gutberlet

Solid and Liquid Interfaces Studied with Neutron Reflectometry

EMPA, Dübendorf, Switzerland, March 16, 2006

T. Gutberlet

Requirements for deuterated biological macromolecules at PSI

DLAB (JRA7) Public session, MPI Martinsried, Germany, March 22-23, 2006

T. Gutberlet

TOF reflectometers at continuous/pulsed sources

ESS-S Workshop on Long Pulse Instrumentation, Lund, Sweden, April 20-21, 2006

T. Gutberlet

Probing Biomembranes at Interfaces Studies with Neutron Reflectometry

Seminar "Complnt", TU Muenchen-Garching, Germany, May 19, 2006

P. Hautle

Polarised solid targets at PSI: recent developments

3rd meeting 'Polarized Nucleon Targets for Europe' in the 6th European Framework Program, Rech, Germany, February 2-4, 2006

P. Hautle

Polarised Neutrons and Polarised Nuclei

Joint Swiss-Russian Workshop on Quantum Magnetism and Polarised Neutrons

Paul Scherrer Institute, March 1-4, 2006

D. Herlach

The PSI-S μ S Facility – current status and perspective,
First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,
September 28 - 30, 2006, Tsukuba, Japan

D. Herlach

The high magnetic field μ SR project at PSI – status and prospects,
First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,
September 28 - 30, 2006, Tsukuba, Japan

D. Herlach

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Workshop on the future development of European muon sources,
November 2-3, 2006, Abingdon, Oxfordshire, United Kingdom

M. Kenzelmann

Konkurrierende Spinwechselwirkungen in Quantenmagneten und in komplexen Materialien
Department of Physics, TU Dresden, Germany, March 29, 2006, seminar

Kenzelmann

The symmetry of multiferroic behaviour in complex transition metal oxide materials
Department of Physics, Oxford University, UK, May 4, 2006, seminar

M. Kenzelmann

Ferroelectric order induced by different magnetic ground states
Theoretical and Experimental Magnetism Meeting, Abingdon, UK, August 4, 2006, Workshop talk

M. Kenzelmann

Magnetic inversion symmetry breaking in multiferroic transition metal oxides
Highly Frustrated Magnetism, Osaka, Japan, August 18, 2006, conference talk

J. Kohlbrecher

SANS with polarized neutrons
IFF Jülich, Germany, January 31, 2006, seminar talk

J. Kohlbrecher

SANS with polarized neutrons for characterization of nanosystems
University of Zaragoza, Spain, February 28, 2006, seminar talk

J. Kohlbrecher

Introduction to small-angle scattering
PSI Summer School Zuoz, Switzerland, August 2006, seminar talk

J. Kohlbrecher

Advantages of global fitting procedures for structural analysis in SAS
IFF Jülich, Germany, September 2006, seminar talk

J. Kohlbrecher, R. Vavrin, A. Wilk, G. Meier, J. Buitenhuis, M.P. Lettinga

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Dynamic nuclear polarization experiments on the protons and ¹³C nuclei in frozen glycine solutions

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Neutron Imaging as Tool for Material Research and Industrial Applications

Indiana University, Bloomington (USA), Oct. 13th 2006

E. Lehmann

Neutron Imaging as Tool for Material Research and Industrial Applications

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Recent experiences from the study of museum objects with neutrons

Int. Workshop within the COST-action G8, Cyprus, May 18th 2006

E. Lehmann

Modern Techniques in Neutron Imaging

Lecture in the Advanced Course for Restorations, La Chaux de Fonds, February 14th, 2006

E. Lehmann

The experimental program for neutron imaging at PSI,

Int. Workshop on Imaging and Neutrons, Oak Ridge (USA), Oct. 23th 2006

E. H. Lehmann, D. Mannes, P. Niemz,

Neutron and X-ray imaging in wood research

Int. Conf. On „Wood Structure and Properties”, Zvolen (Slovakia), Sept. 5th 2006

E. Lehmann

Modern methods in neutron imaging and their use in material research

FZ Karlsruhe, Nov. 24th 2006

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Lessons learned from the non-destructive investigations of museums objects with neutrons and X-rays,

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Options, performance and limitations of neutron imaging systems,

Summer School Zuoz, Aug. 22nd, 2006

H. Luetkens,

Low energy muons: A new probe for magnetism and superconductivity in thin films,

24th May 2006, Institut für Materialwissenschaften, TU Darmstadt, Germany

H. Luetkens

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January 25 – 26, 2006, Paul Scherrer Institute, Villigen, Switzerland

M. Medarde, C. Dallera, M. Grioni, Th. Neisius, J.A. Alonso, M.J. Sayagues and M.T. Casais
 $2Ni^{3+} \rightarrow Ni^{3+\delta} + Ni^{3-\delta}$ charge disproportionation in $RNiO_3$ perovskites (R =rare earth): Implications for the stability of the magnetic structure
Seminar, Laboratorium für Neutronenstreuung, ETH Zürich and PSI Villigen, Villigen, Switzerland, May 18, 2006

J. Mesot
Status and foreseen upgrades of the hybrid TOF spectrometer FOCUS at SINQ
Polarized Inelastic Neutron Scattering (PINS) Workshop, Brookhaven, USA, April 5-8, 2006

J. Mesot
Interplay between electronic and magnetic degrees of freedom in 3d-metal oxides
International Workshop on Self-Organized Strongly Correlated Electron Systems, Seillac, France, May 28-June 1, 2006

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Testing Fermi Liquid Descriptions of Cuprates Superconductors by Means of Momentum Resolved Probes
Séminaire du Département de la Matière Condensée (DPMC), Genève, Switzerland, June 16, 2006

J. Mesot
Neutron and Photon Spectroscopies of Highly Correlated Electron Systems
Rencontres LLB/Soleil: électrons fortement corrélés, Saclay, France, June 22-23, 2006

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Momentum Resolved Neutron and ARPES Investigations of HTSC
Conference on Low Energy Electrodynamics in Solids (LEES06), Tallinn, Estonia, July 2-6, 2006

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Neutron Scattering Investigations of the Abrikosov State of High-Temperature Superconductors
8th International Conference on Materials and Mechanisms on Superconductivity (M2S-HTSC VIII), Dresden, Germany, July 9-14, 2006

J. Mesot
Neutron scattering of low-dimensional systems
Workshop on Polarized Neutrons in Condensed Matter Investigations (PNCMI 2006), Berlin, Germany, September 25–28, 2006

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Proximity effects in metal-superconductor bilayers
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Depth dependent studies of magnetic and superconducting properties in thin films,
Swiss Physical Society,
February 14, 2006, Lausanne

E. Morenzoni,
Depth dependent studies of magnetic and superconducting properties with polarized muons
Triumf, University of British Columbia,
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Depth dependent studies of magnetic and superconducting properties with polarized muons: I,
First Swiss-Japanese workshop on the applications and on new developments in muon
spectroscopy on novel materials,
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E. Morenzoni,
Advanced μ SR techniques
Workshop on the future development of European muon sources,
November 2-3, 2006, Abingdon, Oxfordshire, United Kingdom

F.M. Piegsa
*The nd-Experiment a high-accuracy experiment to measure the spin-dependent neutron-
deuteron scattering length $a_{i,d}$*
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T. Prokscha
Energy dependence of muonium formation in insulators and semiconductors,
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T. Prokscha
Status of the low-energy muon project (LEM) at PSI and overview of experimental program,
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Muonium formation in insulators and semiconductors at low implantation energies,
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T. Prokscha
The high-intensity surface muon beam μ E4 for low-energy muon applications,
First Swiss-Japanese workshop on the applications and on new developments in muon
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September 28 - 30, 2006, Tsukuba, Japan

B. Roessli, S.N. Gvasaliya, M. Janoschek, L. Keller, K. Conder, E. Pomjakushina
Magnetic Properties of $YMnO_3$ Investigated by Elastic and Inelastic Neutron Scattering
The 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity, University of Tsukuba, Japan,
May 15-19, 2006

H.M. Ronnow et al.
Blade Runner - from Risø to PSI and beyond -
TAS Meeting, Rencurel, France, March 11, 2006

H.M. Ronnow et al.
Exploring novel quantum magnets - advent of IN8c and prospects for multiplexing
ILL millennium symposium, Grenoble, France, April 28, 2006

H. M. Ronnow et al.

Exploring novel quantum magnets - a CuTe story and prospects for multiplexing
American Conference on Neutron Scattering, Illinois, USA, June 21, 2006

H.M. Ronnow et al.

The quasi-particle zoo ! - magnetic excitations in spin ladders
Theoretical and Experimental Magnetism Meeting, Abbingdon, UK, August 4, 2006

H.M. Ronnow et al.

Simulations for the new EIGER spectrometer at PSI
MC-Workshop, PSI, Switzerland, October 4, 2006

D. Schaniel, T. Woike, J. Schefer, K. W. Krämer, H. U. Güdel
Photocrystallography with neutrons - Light-induced nitrosyl linkage isomers in sodiumnitroprusside
8th SINQ User Meeting, PSI Villigen, Villigen, Switzerland, May 10, 2006, talk

J. Schefer, M. Boehm B. Roessli, A.S. Wills, B. Ouladdiaf, E. Lelièvre-Berna, U. Staub, C. Baines, G.A. Petrakovskii
Complex Magnetic Ground State of CuB₂O₄
ILL Millennium Symposium & European User Meeting, Europe, Grenoble, France, April 27-29, 2006, talk

J. Schefer

Highlights and Developments at the Swiss Neutron Spallation Source SINQ
Annual Meeting of the Swiss Society for Crystallography, Berne, October 20, 2006, talk

R. Scheuermann

Local environment and dynamics of guest molecules in soft matter structures,
First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,
September 28-30, 2006, Tsukuba, Japan

R. Scheuermann

Avalanche microchannel photodiodes – a new type of photodetectors for the next generation of μ SR spectrometers,
First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,
September 28-30, 2006, Tsukuba, Japan

J. Stahn

A neutron polariser based on magnetically remanent Fe/Si supermirrors
ILL, Grenoble, France, January 18, 2006, seminar

J. Stahn

Antiphase magnetic proximity effect in perovskite superconductor /ferromagnet multilayers
SFB 491 Seminar, Bochum, Germany, February 23, 2006

J. Stahn

Elliptic beam guide - concept and first tests
and
A neutron polariser based on magnetically remanent Fe/Si supermirrors
Workshop on neutron optics, ILL, Grenoble, France, April 26, 2006

J. Stahn
NR in superconductivity - Antiphase magnetic proximity effect in superconductor / ferromagnet multilayers
ADAM user meeting, Bochum, Germany, May 19, 2006

A. Stoykov
Negative muon spin rotation study of acceptor centers in SiC,
XL. PNPI Winter School,
February 15-19, 2006, Repino, Russia

A. Stoykov
Development of scintillation detectors based on avalanche microchannel photodiodes,
1st European Conference on Molecular Imaging Technology,
May 9-12, 2006, Marseille, France, poster.

Th. Strässle, S. Klotz
Neutron scattering under pressure using the paris-edinburgh press
μSR Workshop on High-Pressure Techniques, Villigen PSI, Switzerland, January 25, 2006

Th. Strässle et al.
High-resolution angular dispersive neutron diffraction studies using the Paris-Edinburgh presses
APEC 2006, Applications of Paris-Edinburgh Cells, Paris, France, April 20-21, 2006

Th. Strässle, F. Juranyi, S. Janssen, U. Filges, L. Holitzner, J. Mesot
The time-of-flight spectrometer FOCUS - a versatile instrument at a steady-state neutron source
WINS workshop, Berlin, Germany, September 29-30, 2006

A. Suter
Spin freezing in underdoped HTC's
μSR User Meeting BVRA 2006,
January 25 – 26, 2006, Paul Scherrer Institute, Villigen, Switzerland

A. Suter
Depth dependent studies of magnetic and superconducting properties with polarized muons: II,
First Swiss-Japanese workshop on the applications and on new developments in muon spectroscopy on novel materials,
September 28-30, 2006, Tsukuba, Japan

P. Tregenna-Piggott, P. Allenspach, F. Juranyi
The new time-offlight backscattering spectrometer MARS at SINQ
WINS, Berlin, Germany, September 29-30, 2006

B. van den Brandt, P. Haulte, J. Kohlbrecher, J.A. Konter, S. Mango, H. Glättli, E. Leymarie, E.I. Bunyatova, H. Jouve, H.B. Stuhmann, O. Zimmer
Dynamic Nuclear Polarisation and its application to SANS
Small-Angle Scattering Conference SAS2006, July 7-14, 2006, Kyoto, Japan

S. Van Petegem
MRS-fall meeting Boston, Symposium FF: Processing-Structure-Mechanical Property Relations in Composite Materials, Nov 27 – Dec 1, 2006 (tutorial)

H. Van Swygenhoven
EU-India thematic workshop, "Computational Materials Science",
Bangalore February 20-22, 2006, invited as expert from EU.

H. Van Swygenhoven
MRS spring meeting, San Francisco, April 17-21, 2006 .

H. Van Swygenhoven
EPFL-Séminaire IPMC, Mai 23rd 2006 (Invited seminar)

H. Van Swygenhoven
International Conference on the Strength of Materials (ICSMA14), June 4th to 9th, 2006, in Xi'an city, China (keynote).

H. Van Swygenhoven
NANO2006, Bangalore, August 20-25th 2006

H. Van Swygenhoven
MRS-spring meeting, Symposium "Nanoscale Materials and Modeling", Boston, December 2006, December .

H. Van Swygenhoven
Int. symposium "From microstructure towards plastic behavior of single- and multiphase materials", October 26-27th 2006, Liege, Belgium

H. Van Swygenhoven
Joint EU-China Thematic Workshop "Nanomaterials", November 6-8th 2006, Brussels

H. Van Swygenhoven
MRS Fall meeting, Boston, Nov-27-Dec1, 2006 .

H. Van Swygenhoven
Symposium in honour of Prof. S. Suresh (dean of the Materials Department MIT) on the occasion of his receiving the Acta Materialia Gold Medal, MIT Dec 28-29,

H. Van Swygenhoven
Int. workshop on Nanomaterials workshop on Nanomaterials, Poitiers, Dec 12-13

W. Wagner, Y. Dai, H. Glasbrenner
Materials irradiation facilities at the high-power Swiss proton accelerator complex
TMS2006 Annual Meeting, Wechsler Symposium, San Antonio, TX (USA), 12.-16. 3. 2006

W. Wagner, Y. Dai, H. Glasbrenner
Micromagnetism in a nanophase alloy studied by Small Angle Neutron Scattering
TMS2006 Annual Meeting, Wechsler Symposium, San Antonio, TX (USA), 12.-16. 3. 2006

W. Wagner
Micromagnetism studied by Small Angle Neutron Scattering
Argonne Natl. Lab, Argonne, IL (USA), MSD-Seminar, 16. 5. 2006

W. Wagner
First experience with the MEGAPIE liquid metal target operation at SINQ
IWSMT 06: Eighth International Workshop on Spallation Materials Technology, Taos, NM (USA), 16.-20. 10. 2006

W. Wagner
The MEGAPIE liquid metal target of SINQ – a future option for high-flux spallation neutron source
ILL Scientific Outing 2006, Vogüé (F), 22. 10. 2006

W. Wagner, E. Lehmann, M. Grosse, J. Kohlbrecher
The potential of neutrons of industrial research – Examples from SINQ illustrating opportunities and challenges
ACNS 2006: American Conf. On Neutron Scattering, Chicago, IL (USA), 18.-22.6.2006

W. Wagner
Die Schweizer Spallations-Neutronenquelle SINQ – Eine Nutzereinrichtung mit Entwicklungspotential
Techn. Univ. München (D), TUM-Seminar, 30. 10. 2006

W. Wagner
Ancillary Systems Design: Lessons Learned
MEGAPIE Test International Workshop, Aix en Provence (F), 29. – 30.11.06

U. Zimmermann,
A new general purpose decay-channel spectrometer for high pressure μ SR studies at PSI,
High-Pressure PSI Workshop " μ SR Techniques and Applications"
January 25, 2006, Villigen PSI, Switzerland

CONFERENCE, WORKSHOP AND SEMINAR CONTRIBUTIONS

K. Clausen

Neutron sources

PSI Summer School on Condensed Matter Research Neutron, X-ray and Muon Studies of Nano Scale Structures August 19-26, 2006

K. Clausen

Neutron sources and instrumentation

SISN summer school Sirolo, Ancona, Italy, 26-28 June 2006

K. Clausen

A new Era for research based on the use of neutron scattering

Odense University, Denmark, 7 march 2006

K. Clausen

Future activities at PSI on liquid / solid spallation targets

MEGAPIE-TEST International Workshop on heavy liquid metal spallation targets for transmutation Aix en Provence, November 29-30, 2006

A. Comment, F. Kurdzesau, S. Jannin, J. van der Klink, P. Hautle, B. van den Brandt

C-13 DNP of sodium acetate and glycine in frozen liquid solutions

Swiss Physical Society Jahrestagung.- Lausanne, February 13-14, 2006, contributed ID 225

A. Comment, F. Kurdzesau, S. Jannin, J. van der Klink, P. Hautle, B. van den Brandt

Large sensitivity enhancement of carbon-13 magnetic resonance by dynamic nuclear polarization to study brain metabolism

7-th International Conference on Brain Energy Metabolism. Integrating molecular, cellular and metabolic aspects of neuron-glia interactions.- Lausanne, August 15-18, 2006, poster

K. Conder, M. Stingaciu, E. Pomjakushina, A. Podlesnyak

Structural, magnetic and transport properties of layered cobaltites $LnBaCo_2O_{5+x}$

International Conferences on Modern Materials and Technologies (CIMTEC 2006), Acireale, Sicily, Italy, June 4-9, 2006, oral presentation

K. Conder, A. Podlesnyak, E. Pomjakushina, V. Pomjakushin, M. Stingaciu, A.E. Karkin

Transport properties and oxygen isotope effect in layered cobaltites $RBaCo_2O_{5+x}$

International Conference on Magnetism (ICM 2006), Kyoto, Japan, August 20-25, 2006, poster presentation

U. Filges, G. Zsigmond, J. Saroun

McStas/VITESS/Restrax intercomparison for the TOF Instrument FOCUS

MCNSI-meeting, Risoe, Denmark, February 21-22, 2006, contributed

U. Filges, P. Allenspach, M. Hagen

Simulations for the HYSPEC polarization option

International Workshop on Applications of Advanced Monte Carlo Simulations in Neutron Scattering, Villigen PSI, October 3-4, 2006, contributed

J. Gironnet

Recherche de matière noire par bolomètres massifs scintillants

during a nuclear physics school called "De la Physique au Détecteur", in Bénodet in France, November 15-23, 2006

J. Gironnet

Possibilités au PSI

during a scintillating cryodetector meeting at the Nuclear Physics Institute of Lyon, in Lyon in France, December 14, 2006

H. Grimmer

The effect of crystal symmetry on the spectral decomposition of the linear elastic tensor

14. Jahrestagung der Deutschen Gesellschaft für Kristallographie, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany, April 3-6 2006, poster

H. Grimmer

The effect of crystal symmetry on the spectral decomposition of the linear elastic tensor

Annual Meeting 2006 of the Swiss Society for Crystallography, Universität Bern, Bern, Switzerland, October 20, 2006, poster

S. Jannin, F. Kurdzesau, A. Comment, J. van der Klink, P. Hautle, B. van den Brandt

C-13 DNP of sodium acetate and glycine in frozen liquid solutions

Euromar. Magnetic resonance for the Future.- York, England, July 16-21, 2006, poster HS4.

M. Janoscheck, M. Medarde, J. Rodríguez-Carvajal and B. Roessli

Spherical Neutron Polarimetry Analysis with FullProf: soon a reality

Annual Meeting of the Swiss Society for Crystallography, Bern, Switzerland, October 20, 2006, poster

M. Koennecke, U. Filges

Integration of McStas Simulations into the Instrument Control Software SICS

NOBUGS 2006, Berkeley, USA, October 2-4, 2006, USA, poster

F. Kurdzesau, S. Jannin, A. Comment, J. van der Klink, P. Hautle, T. Konter, Ben van den Brandt

13C DNP of sodium acetate and glycine in frozen liquid solutions

EUROMAR 2006 (EENC-Ampère-NMR-DG), York, United Kingdom, July 16-21, 2006, poster

F. Kurdzesau, S. Jannin, A. Comment, J. van der Klink, P. Hautle, T. Konter, B. van den Brandt

13C DNP of sodium acetate and glycine in frozen liquid solutions

5th PSI Summer School on Condensed Matter Research, Lyceum Alpinum, Zuoz, Switzerland, August 19–26, 2006, poster

F.M. Piegsa

The nd-Experiment a high-accuracy experiment to measure the spin-dependent neutron-deuteron scattering length $a_{i,d}$

Laboratory for Particle Physics (LTP) – Paul Scherrer Institut, Villigen PSI, Switzerland, January 18, 2006, seminar

E. Pomjakushina, K. Conder, M. Stingaciu, V. Pomjakushin, A. Podlesnyak, D. Chernyshov

Metal-Insulator Transition in Layered Cobaltites $R\text{BaCo}_2\text{O}_{5.5}$

European Powder Diffraction Conference (EPDIC 2006), Geneve, Switzerland, August 31-September 4, 2006, oral presentation

J. Stahn, M. Koennecke, T. Gutberlet

AMOR – a versatile time-of-flight polarized neutron reflectometer at SINQ/PSI

SNI2006, Hamburg, Germany, October 4-6, 2006, poster

S. Streule, M. Medarde, A. Podlesnyak, E. Pomjakushina, K. Conder, S. Kazakov, J. Karpinski, J. Mesot
Short-range charge ordering and ferromagnetism-antiferromagnetism competition in $\text{Ho}_{0.1}\text{Sr}_{0.9}\text{CoO}_{3-x}$ ($0.15 \leq x \leq 0.49$)
10th European Powder Diffraction Conference, EPDIC 10, Geneva, Switzerland, September 1-4, 2006, contributed

G. Theidel, M. Koennecke
Histogram Memory Computer with Linux/RTAI and Integrated WWW server
NOBUGS 2006, Berkeley, USA, October 2-4, 2006, poster

J. P. Urrego-Blanco, C. R. Bingham, B. van den Brandt, A. Galindo-Uribarri, J. Gómez del Campo, P. Hautle, J. A. Konter, E. Padilla-Rodal, F. Piegsa, P. Schmelzbach
Recent Progress in the Development of a Polarized Target for Reactions with Radioactive Ion Beams
Nuclear Structure '06, Oak Ridge TN, USA, July 26-28, 2006

J.P. Urrego-Blanco, C.R. Bingham, B. van den Brandt, A. Galindo-Uribarri, J. Gómez del Campo, P. Hautle, J.A. Konter, E. Padilla-Rodal, F. Piegsa, P.A. Schmelzbach
Recent progress in the development of a polarized target for reactions with radioactive ion beams
5th PSI Summer School on Condensed Matter Research, Lyceum Alpinum, Zuoz, Switzerland, August 19–26, 2006, poster

J. P. Urrego-Blanco, C. R. Bingham, B. van den Brandt, A. Galindo-Uribarri, J. Gómez del Campo, P. Hautle, J. A. Konter, E. Padilla-Rodal, P. A. Schmelzbach
Recent progress in the development of a polarized proton target for reactions with radioactive ion beams
CAARI 2006: 19th International Conference on the Application of Accelerators in Research and Industrie, Fort Worth, Texas USA, August 20-25, 2006

J.P. Urrego-Blanco
Development of polarized proton targets for reactions with radioactive ion beams
University of Tennessee, Knoxville, October 16, 2006, seminar

B. van den Brandt, P. Hautle, J. Kohlbrecher, J.A. Konter, F.M. Piegsa, J.P. Urrego-Blanco, H. Glättli, H. Griebshammer, O. Zimmer
The nd-Experiment a high-accuracy experiment to measure the spin-dependent neutron-deuteron scattering length $a_{i,d}$
3rd meeting 'Polarized Nucleon Targets for Europe' in the 6th European Framework Program, Rech, Germany, February 2-4, 2006

B. van den Brandt, H. Glättli, H. Griebshammer, P. Hautle, J.A. Konter, F.M. Piegsa, J. P. Urrego-Blanco, O. Zimmer
An Accurate Measurement of the Spin Dependent Neutron-Deuteron Scattering Length
SPIN 2006, the 17th International Spin Physics Symposium, Kyoto, Japan, October 2-7, 2006, contributed talk

M. Zolliker, M. Koennecke
SEA – a Modular Sample Environment Control System
Fourth International Workshop On Sample Environment at Neutron Scattering Facilities, Argonne, USA, September 6-8, 2006, contributed talk

J. O. Birk, K. H. Klenø, K. Lefmann, P. Willendrup
A simulation-based home page for high-school level education
PSI simulation workshop October 2006, poster

- Y. Bodenthin, G. Schwarz, Th. Geue, D.G.Kurth, U. Pietsch
Structure driven remanent high-spin state in metallocsupramolecular assemblies
 25th User Meeting Bessy December 5-9, Germany, poster
- S. Busch, F. Juranyi, T. Gutberlet
Dynamics in model membrane systems
 Jahrestagung SPG, Lausanne, Switzerland, February 13-14, 2006, poster
- S. Busch, F. Juranyi, T. Gutberlet
Dynamics in model membrane systems
 Workshop on Dynamics of Artificial and Biological Membranes, Gomadingen, Germany, March 20-22, 2006, poster
- S. Busch, F. Juranyi, T. Gutberlet
Water Dynamics in Phospholipid Model Membrane Systems
 SNI2006, Hamburg, Germany, October 4-6, 2006, poster
- S. Busch, F. Juranyi, T. Gutberlet
Water Dynamics in Phospholipid Model Membrane Systems
 QENS2006, Bloomington, IN, USA, June 14-17, 2006, poster
- A. Cervellino, C. Giannini, A. Guagliardi, D. Zanchet, T.C.R. Rocha, M. Ladisa, P.D. Cozzoli, L. Manna
Diffraction Analysis of Exotic-Shaped Nanoclusters
 ICN+T2006- International Conference on Nanoscience and Technology 2006, Basel, Switzerland, July 30-August 4, 2006, contributed talk
- A. Cervellino, L. Keller, U. Filges
Standardless Neutron Powder Diffraction 2D-Detector Calibration
 EPDIC10 – European Powder Diffraction Conference, Geneva, Switzerland, September 1-4, 2006, poster
- J. Chang
High- and low- energy electronic responses in high temperature superconductors
 Anderson Meeting Geneva, Switzerland, September 27, 2006, seminar
- A. Dönni, H. Kitazawa, L. Keller
Geometrically Frustrated Commensurate and Incommensurate Magnetic Structures TbPd_{0.9}Ni_{0.1}Al Studied by Powder Diffraction
 QuBS2006, Tokai, Japan, August 28-30, 2006, poster
- A. Dönni, H. Kitazawa, L. Keller
Neutron Diffraction Study of Geometrically Frustrated System TbPd_{1-x}Ni_xAl (x= 0, 0.1)
 Meeting of the Physical Society of Japan, Chiba, Japan, September 23-26, 2006, poster
- A. Dönni, H. Kitazawa, T. Goto, Y. Nemoto, L. Keller
Neutron Scattering Experiments on R₃Pd₂₀X₆ (X=Ge, Si) Compounds
 Meeting of the Neutron Scattering Society of Japan, Tokai, Japan, December 5-6, 2006, poster
- J.L. Gavilano, B. Pedrini, K. Magishi, J. Hinderer, M. Weller, H.R. Ott, S.M. Kazakov, J. Karpinski
Localized Versus Itinerant Moments in Na_{0.7}CoO₂
 2006 Swiss Physical Society - MaNEP meeting □ Lausanne, Lausanne, Switzerland, February 13-14, 2006, poster

J.L. Gavilano, B. Pedrini, M. Weller, J. Hinderer, H.R. Ott, S.M. Kazakov, J. Karpinski
Itinerant Versus Localized Spins in Na_xCoO₂
Joint Swiss-Russian Workshop on Quantum Magnetism and Polarized Neutrons, Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen PSI, Switzerland, March 1-4, 2006, oral contribution

J.L. Gavilano
Some Open Issues in the Magnetism of Na_xCoO₂
First International Workshop on the Physical Properties of Lamellar Cobaltates, Université Paris-Sud, Orsay, France, July 16-19, 2006, oral contribution

Th. Geue, P. Huber, B. Reinhold, K. Morawetz, U. Pietsch, M. Textor
Template-assisted formation of ordered colloidal assemblies
X-Top 2006, Baden-Baden, Germany, September 19-22, 2006, poster

Th. Geue, P. Huber, B. Reinhold, K. Morawetz, J. Grenzer U. Pietsch, M. Textor
Template-directed formation of ordered colloidal assemblies
SNI 2006, Hamburg, Germany, October 4-6, 2006, poster

C. Giannini, A. Cervellino, A. Guagliardi, D. Zanchet, T.C.R. Rocha, M. Ladisa
A Depye Function Based Powder Diffraction Data Analysis Method
EPDIC10 – European Powder Diffraction Conference, Geneve, Switzerland, September 1-4, 2006, contributed talk

A. Guagliardi, A. Cervellino, C. Giannini, D. Zanchet, M. Ladisa
Whole Powder Pattern Methods for Nanoparticles characterization
ECM23 – 23rd European Crystallographic Meeting Leuven, Belgium, August 6.-11, 2006, contributed talk

T. Gutberlet
Lipid Distribution in Model Membrane Systems
μSR Users' Meeting, PSI, Villigen, Switzerland, January 25-26, 2006

T. Gutberlet
Neutron reflectometry as tool to characterize soft matter and biomaterials at SINQ/PSI
Refsans workshop, TU Muenchen-Garching, Germany, September 22, 2006, contributed talk

S. N. Gvasaliya
Cold-neutron three-axis spectrometers by the example of TASP
XL Winter school of St. Petersburg Nuclear Physics Institute, St. Petersburg, Russia, February 13-26, 2006, lecture

S.N. Gvasaliya, B. Roessli, R.A. Cowley, S. Kojima, S.G. Lushnikov
Neutron Scattering Studies of the Low-Frequency Dynamics of 0.68PbMg_{1/3}Nb_{2/3}O₃-0.32PbTiO₃ and PbMg_{1/3}Nb_{2/3}O₃
The 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity, University of Tsukuba, Tsukuba, Japan, May 15-19, 2006, oral

J. í Hjøllum, L. Theil Kuhn, K. Lefmann, A.B. Abrahamsen, B. Lebech, N.H. Andersen, J. Raittila, Ch. Niedermayer, N.B. Christensen, P. Paturi
Neutron scattering investigations of the antiferromagnetic phase of YBCO nano-particles
Danish Physical Society, annual meeting June 2006, Denmark, poster

J. í Hjøllum, L.T. Kuhn, K. Lefmann, J.-C. Grivel, A.B. Abrahamsen, B. Lebech, N.H. Andersen, J. Raittila, Ch. Niedermayer, N. B. Christensen, P. Paturi
Investigations of the antiferromagnetic phase of YBCO nano-particles
Correlated electron workshop on Crete, October-November 2006, poster

T. Hong, M. Kenzelmann, M. Bouloubasis, D. Reich, C. Broholm
Field-Induced Quantum Criticality in a Two-Dimensional Antiferromagnet
APS March Meeting, Baltimore, Md, USA, March 13-17, 2006

F. Juranyi, F. Gonzalez, S. Gvasaliya
Geometrical aspects of QENS experiments in case of anisotropic samples
CONFIT, ILL, Grenoble, France, March 24-26, 2006, Poster

F. Juranyi, T. Straessle, L. Holitzner, N. Schlumpf, U. Greuter, Th. Gahl, S. Janssen, J. Mesot, R. Hempelmann
Der neue 2D Kleinwinkeldetektor des Flugzeitspektrometers FOCUS, SINQ
SNI, Hamburg, Germany, October 4-6, 2006, poster

L. Keller, U. Filges
Design of a Neutron Powder Diffractometer at SINQ using Monte Carlo Simulations
European Powder Diffraction Conference, EPDIC10, Geneva, Switzerland, September 1-4, 2006, poster

H. Kitazawa, A. Dönni, L. Keller, P. Fischer, J. Prchal
Isostructural phase transitions in $TbPd_{1-x}Ni_xAl$ ($x=0, 0.1$)
Meeting of the Neutron Scattering Society of Japan, Tokai, Japan, December 5-6, 2006, poster

K. H. Klenø, K. Lefmann, R. Bewley, P. Willendrup, P. Christiansen
Effect of chopper jitter on proposed LET instrument at ISIS target station 2
PSI simulation workshop October 2006, poster

R. Krastev, T. Gutberlet, N. Mishra, A. Wildes, V. Lauter-Pasyuk
Neutron Specular Reflection and Off-specular Scattering from Free Standing Liquid Foam Films
ILL Millennium Symposium and European Users Meeting, April 27-29, 2006, poster

R. Krastev, T. Gutberlet, N. Mishra, A. Wildes, V. Lauter-Pasyuk
Neutron Specular Reflection and Off-specular Scattering from Free Standing Liquid Foam Films
ILL Softmatter User Meeting, ILL/ESRF Grenoble, France, November 22-24, 2006, poster, contribution talk

K. Lefmann
Neutron MC simulations for ESS Software, reliability, and visions
ESS Workshop, Lund April 2006, talk

K. Lefmann et al.
Virtual experiments for tomorrows neutron science
PSI simulation workshop, October 2006, talk

K. Lefmann
Neutron scattering Possibilities for Chemistry
Facilities for Danish users and Future plans, Institute of Chemistry, University of Copenhagen, November 2006, talk

T. Lin, J. Wu, U. Jeng, H. Lee, N. Torikai, T. Gutberlet
Neutron and X-ray Reflectivity Studies of Enhanced DNA Adsorption by DC-Cholesterol Monolayer with Ions
ACNS 2006, St. Charles, IL, USA, June 18-22, 2006, poster

J. Mesot
Description of the Instrumentation at SINQ
Quantum Magnetism and Polarized Neutrons Workshop, PSI Villigen, Switzerland, February 28-March 4, 2006

J. Mesot

Continuous vs spallation neutron sources

International Summer School on Neutron Techniques in Molecular Magnetism", Jaca, Spain, August 31-September 9, 2006, lecturer

J. Mesot

Elementary scattering

5th PSI Summer School on Condensed Matter Research: Neutron, X-ray and Muon Studies of Nano Scale Structures, Zuzo, Switzerland, August 19-26, 2006, lecturer

J. Mesot

Neutron- and photon-based spectroscopies

Second MaNEP summer school: Probing the Physics of Low Dimensional Systems, Saas-Fee, Switzerland, September 11-16, 2006, lecturer

K. Morawetz, B. Stiller, Th. Geue, M. Saphiannikova, Ullrich

Patterning in Azobenzene Polymer Films

Spring-Meeting of the German Physical Society, Berlin, Germany, March 6-9, 2006, poster

K. Mortensen

Block Copolymer Melts and Networks Shear-Induced Texture and Shear-Induced Phase Transitions

2006-Annual Meeting in the Bio- and Nanopolymers Centre of Excellence, Helsinki, Finland, June 6-7, 2006, talk

K. Mortensen, O. Hassager, J. K. Nielsen, A. Bach, K. Almdal

Time Resolved Structural Changes and Relaxations in Polymer Melts Exposed to Elongational Extension and Shear

XIII International Conference on Small-Angle Scattering, Kyoto, Japan, July 9-13, 2006, talk

Ch.M. Papadakis, R. Ivanova, K. Lüdtkke, K. Mortensen, P.K. Pranzas, R. Jordan

Micellar structure of amphiphilic poly(2-oxazoline) diblock copolymers. SAS-Kyoto

XIII International Conference on Small-Angle Scattering, Kyoto, Japan, July 9-13, 2006, talk

G. Petrakovskii, N. Volkov, G. Abramova, J. Schefer, H. Szymczak, V. Sokolov

New layered 3d-materials for spintronics

Workshop INTAS – Siberian Branch Of the Russian Academy of Sciences, Novosibirsk, Russia, May 10-12, 2006, poster

V. Pomjakushin

Effect of oxygen isotope substitution on magnetic ordering and phase separation in $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$

8th SINQ Users Meeting, Paul Scherrer Institut, Villigen PSI, Switzerland, May 10, 2006, oral

V. Pomjakushin, A. Balagurov, K. Conder, E. Pomjakushina, D. Sheptyakov,

Effect of oxygen isotope substitution and crystal micro-structure on magnetic ordering and phase separation in $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$

10th European Powder Diffraction Conference (EPDIC), University of Geneva, Switzerland, September 1-4, 2006, poster

B. Reinhold, Th. Geue, U. Petsch, P. Bösecke

Ultra-small angle x-ray scattering at colloidal crystals on pre-patterned support

Spring-Meeting of the German Physical Society, Berlin, Germany, March 6-9, 2006, contributed talk

- H.M. Ronnow et al.
Polarons and electronic confinement in a layered manganite
 International Conference on Magnetism, Kyoto, Japan, August 24, 2006, poster
- D. Schaniel, T. Woike, J. Schefer, K. W. Krämer, H. U. Güdel
LICHTINDUZIERTE ISONITROSYL-KONFIGURATION IN $Na_2[Fe(CN)_5NO] \cdot 2 H_2O$
 Deutsche Kristallographische Gesellschaft (DGK), Freiburg, Germany, April 3-6, 2006, poster
- D. Schaniel, T. Woike, J. Schefer, V. Petricek, K. W. Krämer, H. U. Güdel
Photocrystallography with neutrons - Light induced structural changes in $Na_2[Fe(CN)_5NO] \cdot 2 H_2O$
 23rd European Crystallographic Meeting, Leuven, Belgium, August 6-11, 2006, talk
- D. Schaniel, T. Woike, J. Schefer, P. Fertey, N.K. Hansen, V. Petricek
The modulated structure of the holographic data storage material $Sr_xBa_{1-x}Nb_2O_6$
 23rd European Crystallographic Meeting, Leuven, Belgium, August 6-11, 2006, poster
- M. Schneider
Incommensurate magnetic modulations in the magnetic superconductor $HoNi_2^{11}B_2C$ studied by Neutron Scattering
 International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors, Dresden, Germany, July 9–14, 2006, talk
- D. Sheptyakov, K.M. Mogare, R. Bircher, H.-U. Güdel, M. Jansen
Neutron diffraction study of the crystal and magnetic structures of Na_2RuO_4
 10th European Powder Diffraction Conference (EPDIC-10), Genève, Switzerland, September 1-4, 2006, contributed
- H. Shigematsu, Y. Akishige, S.N. Gvasaliya, V.Yu. Pomjakushin, S.G. Lushnikov, S. Kojima
Neutron Power Diffraction Study of the Phase Transition in $BaTi_2O_5$
 The 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity, University of Tsukuba, Tsukuba, Japan, May 15-19, 2006, poster
- J. Stahn, Ch. Niedermayer, H.-U. Habermeier, J. Chakhalian, B. Keimer, Ch. Bernhard, J. Hoppler
Interface magnetisation in a high- T_c superconductor / ferromagnet multilayer
 PNCMI 2006, Berlin, Germany, September 25-28, 2006, poster
- J. Stahn
Antiphase magnetic proximity effect in perovskite superconductor / ferromagnet multilayers
 SNI 2006, Hamburg, Germany, October 4-6, 2006, contributed
- J. Stahn, M. Koennecke, T. Gutberlet
AMOR – a versatile time-of-flight polarized neutron reflectometer at SINQ/PSI
 SNI2006, Hamburg, Germany, October 4-6, 2006, poster
- P. Szewczykowski, F. Guo, R.H. Berg, S. Ndoni, K. Mortensen, M.E. Vigild
Nano-Porous Elastomers based on Polymer Self-Assembly
 Nordic Polymer Days, May 29-33, 2006, talk
- B. Thielemann, Ch. Rüegg, H.M. Rønnow, J. Stahn, J. Mesot, D. F. McMorrow, K.W. Kraemer, H.-U. Guedel
Spin Dynamics in the Organic Quantum Magnet $(C_5H_{12}N)_2CuBr_4$
 Joint Swiss-Russian Workshop on Quantum Magnetism and Polarized Neutrons, Villigen PSI, Switzerland, April 1-3, 2006, contributed

B. Thielemann, Ch. Rüegg, H. M. Rønnow, D. F. McMorrow, J. Mesot, K. W. Krämer, D. Biner, H.-U. Güdel, J. Stahn, K. Habicht, M. Boehm
Spin Dynamics in the Organic Quantum Magnet (Hpip)₂CuBr₄
SINQ User Meeting, Villigen PSI, Switzerland, May 10, 2006, contributed

B. Thielemann, Ch. Rüegg, H. M. Rønnow, D. F. McMorrow, J. Mesot, K. W. Krämer, D. Biner, H.-U. Güdel, J. Stahn, K. Habicht, M. Boehm
Spin Dynamics in the Organic Quantum Magnet (Hpip)₂CuBr₄
Highly Frustrated Magnetism 2006, Osaka, Japan, August 15-19, 2006, contributed poster

B. Thielemann, Ch. Rüegg, H. M. Rønnow, D. F. McMorrow, J. Mesot, K. W. Krämer, D. Biner, H.-U. Güdel, J. Stahn, K. Habicht, M. Boehm
Spin Dynamics in the Organic Quantum Magnet (Hpip)₂CuBr₄
International Conference on Magnetism, Kyoto, Japan, August 20-25, 2006, contributed poster

B. Thielemann
Probing the physics of low dimensional Systems
MaNEP Summer School, Saas-Fee, Switzerland, September 11-16, 2006

L. Udby, K. Lefmann, P. Willendrup, B.O. Wells, H.E. Mohottala, Ch. Niedermayer, N.B. Christensen, E. Farhi
Analysing single-crystal diffraction data using McStas
PSI simulation workshop October 2006, poster

R. Vavrin
Pressure induced phase transitions in sterically stabilised colloids
12th IACIS International Conference on Surface and Colloid Science, Beijing, China, October 15-20, 2006, contributed

M. Weller, J. Hinderer, J.L. Gavilano, H.R. Ott, T. Feher, L. Forro
NMR studies of BaVS₃
2006 Swiss Physical Society - MaNEP meeting □ Lausanne, Lausanne, Switzerland, February 13-14, 2006, oral contribution

S. Weyeneth, J. Hinderer, M. Weller, J.L. Gavilano, E. Felder, F. Hulliger, H.R. Ott
NMR study of CeTe at low temperatures
2006 Swiss Physical Society - MaNEP meeting □ Lausanne, Lausanne, Switzerland, February 13-14, 2006, poster

P. Willendrup, E. Farhi, K. Lieutenant, P. Christiansen, K. Lefmann
New features of McStas, the flexible neutron ray-trace simulation package
PSI Simulation Workshop October 2006, poster

O. Zaharko, H. M. Rønnow et al.
Low Dimensional Magnetism - the LEGO of physics
D-PHYS evaluation, ETH-Zürich, Switzerland, May 17, 2006, poster
O. Zaharko, H. M. Rønnow, K. Prsa
Ground state in spin-tetrahedra systems Cu₂Te₂O₅X₂ (X=Br, Cl)
Highly Frustrated Magnetism, Osaka, Japan, August 15-19, 2006, poster

O. Zaharko, H. M. Rønnow, K. Prsa, J. Mesot, P.J. Brown, H. Berger
Ground state in spin-tetrahedral system Cu₂Te₂O₅X₂ (X=Cl, Br)
International Conference on Highly Frustrated Magnetism 2006, Osaka, Japan, August 15-19, 2006, poster

O. Zaharko

Coupled and isolated Cu²⁺ S=1/2 spin tetrahedral systems studied by neutron scattering
Ljubljana, Slovenija, December 4, 2006, seminar

D. Andreica,

μSR under pressure: the method,
ICM satellite workshop "Novel pressure-induced phenomena in condensed matter systems",
August 26-29, 2006, Fukuoka, Japan

D. Herlach

SμS News

μSR User Meeting BVRA 2006,
January 25 – 26, 2006, Paul Scherrer Institute, Villigen, Switzerland.

H. Luetkens, M. Stingaciu, Y.G. Pashkevich, P. Lemmens, E. Pomjakushina, K. Conder, D. Cheptiakov, H. H. Klauss

Oxygen Isotope Effect and Magnetic Phase Transitions of the Layered Cobaltite RBaCo₂O_{5.5} (R=Y, Ho)

19th International Conference on Magnetism, Kyoto, Japan, 20.-25.8.2006

H. Luetkens, E. Morenzoni, T. Prokscha, D. Eshchenko, G.J. Nieuwenhuys, and A. Suter
Low Energy mSR: A Depth Selective Local Magnetic Probe

19th International Colloquium on Magnetic Films and Surfaces, Sendai, Japan, 14.-18.8.2006

E. Morenzoni,

Direct observation of non-local effects in superconductors

Deutsche Physikalische Gesellschaft Tagung, March 28, 2006, Dresden, Germany.

A. Carminati, A. Kaestner, R. Hassanein, A. Koliji

Hydraulic properties of aggregate-aggregate contacts

Proc. GeoX 2006, 2nd International Workshop on X-Ray CT for Geomaterials

October 4-7, 2006 - Grenoble & Aussois, France

Advances in X-ray Tomography for Geomaterials, Edited by: J. Desrues, G. Viggiani and P.

Bésuelle, pg 325-332, ISBN: 1905209606

F.C. de Beer, N. Kardijlov, R. Hassanein, E. Lehmann

Scattered neutrons and their effect on quantitative neutron radiography

Proc. 8th World conference on neutron radiography, Oct 16-19, 2006, NIST Gaithersburg, USA

F. Groeschel, A. Cadiou, S. Dementjevs, M. Dubs, C. Fazio, T. Kirchner, Ch. Latge, P. Ming, K. Thomsen and W. Wagner

The MEGAPIE project status update – high power liquid metal spallation target

Proc. ICANS-XVII, Santa Fe NM, USA, LA-UR-06-3904, 590 (2006)

C. Grünzweig, F. Pfeiffer, O. Bunk, I. Johnson, X. Donath, G.Frei, E. Lehmann, H. Rønnow, C. David

Neutron Phase Imaging and Tomography

Proc. 8th World conference on neutron radiography, Oct 16-19, 2006, NIST Gaithersburg, USA

R. Hassanein, P. Vontobel, E. Lehmann

Correction software tool for neutron tomography

Proc. 8th World conference on neutron radiography, Oct 16-19, 2006, NIST Gaithersburg, USA

- R. Hassanein, E. Lehmann, P. Vontobel
Investigation of water distribution and flow processes by quantitative neutron tomography
 Multi-scale Modeling of Flow and Transport in Porous Media
 April 7 - 12, 2006, Congress Centre Stefano Franscini, Monte Verita, Switzerland
- A. Kaestner, P. Lehmann, A. Carminati, H. Flühler, E. Lehmann, M. Stampanoni, F. Beckmann
Imaging as a tool to investigate water flow in soil
 Multi-scale Modeling of Flow and Transport in Porous Media April 7 - 12, 2006, Congress Centre Stefano Franscini, Monte Verita, Switzerland
- A. Koliji, A. Carminati, A. Kaestner, L. Vuillet, L. Laloui, H. Fluehler, P. Vontobel, R. Hassanein
Experimental study of flow and deformation in aggregated soils using neutron tomography
 Proc. GeoX 2006, 2nd International Workshop on X-Ray CT for Geomaterials
 October 4-7, 2006 - Grenoble & Aussois, France
 Advances in X-ray Tomography for Geomaterials, Edited by: J. Desrues, G. Viggiani and P. Bésuelle, pg 341-348, ISBN: 1905209606
- A. Koliji, L. Vuillet, L. Laloui, A. Carminati, A. Kaestner, H. Flühler, P. Lehmann, R. Hassanein, E. Lehmann, and P. Vontobel
Structure degradation of dry aggregated soils: Experimental evidence and model formulation
 4th Int. Conf. Unsaturated Soils, UNSAT06. Eds G.A. Miller, C.E. Zappatà, H.S. L., and D.G. Fredlund.
 USA, Vol.2, 2006, p. 2174-2185.
- G. Kuehne, P. Vontobel, G. Frei, E. Lehmann, M. Buehlmann, K.C. Heiniger, B. Zweifel
Neutron imaging facilities at the Paul Scherrer Institute and their application for non-destructive testing of abrasive water-jet nozzles.
 Proc. ECNDT 2006, Sept 25-29, Berlin, Germany, NDT.net - Nov 2006, Vol. 11 No. 11
- E.H. Lehmann, G. Frei, R. Widler, H. Materna, D. Glauser
The inspection of tube fitting systems in use for drinking water supply by means of neutron imaging methods
 Proc. ECNDT 2006, Sept 25-29, Berlin, Germany, NDT.net - Nov 2006, Vol. 11 No. 11
- P. Lehmann, N. Shokri, P. Vontobel and D. Or
Preferential Evaporation in the Presence of Textural Contrasts.
 in Proc.: Preferential flow and transport processes in soil, November 4-9, 2006
 Centro Stefano Franscini, Monte Verità, Ascona, Switzerland
- W.H. Leung, S. Dementjev, M. Dierckx, and F. Groeschel
The Thermal Hydraulic Test of the MEGAPIE Cooling System and System Code Validation
 Proc. of ICAPP '06, Reno, NV USA, June 4-8, 2006, Paper Nr. 6143
- D. Mannes, P. Niemz, E. Lehmann
Investigation of wood properties by means of neutron imaging techniques
 Proc. 6th International PhD Symposium in Civil Engineering, August 23 – 25, 2006, Zurich
- D. Mannes, E. Lehmann, S. Oswald, P. Niemz
Investigation of water transport processes in plants by means of neutron imaging techniques
 Proc. 5th Plant Biomechanics Conference – Stockholm, August 28 – September 1 2006.
- E. Noah, E. Bouquerel, R. Catherall, M. Eller, S. Fernandes, I. Guenther-Leopold, F. Groeschel, A. Kalt, J. Lettrey, E. Manfrin, S. Marzari, T. Stora, R. Wilfinger, and L. Zanini,
TARPIPE: TARget Prototype Irradiations at PSI for EURISOL
 Proc. of the 7th international conference on Radioactive nuclear beams, Cortina d'Ampezzo, Italy, July 3-7, 2006.

- A. Papafotiou, R. Helmig, J. Schaap, A. Kaestner, P. Lehmann, H. Flübler, R. Hassanein, E. Lehmann
Problem identification and sensitivity analysis for a well-controlled 3d lab-scale multistep experiment
 Multi-scale Modeling of Flow and Transport in Porous Media, April 7 - 12, 2006, Congress Centre Stefano Franscini, Monte Verita, Switzerland
- J.A. Patorski, F. Groeschel
Experimental determination of local convection heat transfer coefficient field using two-dimensional and dynamic infrared thermography (2DD-IRT) method
 Proc. of SPIE, Thermosense XXVIII, Volume 6205, ISSN 0277-786X 2006
- J.A. Patorski, F. Groeschel, I. Platnieks
Experimental determination of the local heat transfer coefficient for MEGAPIE target window using infrared thermography
 Proc. of IAEA, Theoretical and Experimental Studies of Heavy Liquid Metal Thermal Hydraulics, IAEA-TECDOC-1520, ISSN 1011-4289, 2006
- B. Robinson, A. Moradi, H. Conesa, S. Roulier, M. Menon, E. Lehmann, R. Schulin.
Preferential flow and the phytomanagement of contaminated sites
 in Proc.: Preferential flow and transport processes in soil, November 4-9, 2006
 Centro Stefano Franscini, Monte Verità, Ascona, Switzerland
- M. Vasin, I. Neuweiler, P. Lehmann, H. Flübler, R. Hassanein, E. Lehmann
Influence of soil structure on flow of water and air – Experimental study
 Multi-scale Modeling of Flow and Transport in Porous Media, April 7 - 12, 2006, Congress Centre Stefano Franscini, Monte Verita, Switzerland
- R. van Langh, D. Visser, P. Vontobel, M. Estermann, E.H. Lehmann, W. Kockelmann
A neutron tomography and tome of flight diffraction study of early renaissance sculptures. A new tool for art historians.
 Proc. 8th World conference on neutron radiography, Oct 16-19, 2006, NIST Gaithersburg, USA
- D. Visser, R. van Langh, P. Vontobel, E. Lehmann
From Vulcan's Forge : Neutron Tomographic Investigations of Early Italian and Northern Renaissance Bronze Sculptures from the Rijksmuseum Amsterdam
 36th Int. Symp. on Archaeometry (ISA 2006), May 2nd - 6th, 2006 Quebec City, Canada.
- P. Vontobel, R. Hassanein, A. Carminati, A. Kaestner, P. Lehmann, A. Koliji, P. Christe
Neutron imaging for soil physics and Geology at Paul Scherrer Institute.
 Proc. 8th World conference on neutron radiography, Oct 16-19, 2006, NIST Gaithersburg, USA
- P. Vontobel
Neutron imaging for soil physics
 FRM II Workshop Neutrons For Geoscience, Jul 14, 2006, Technical University Munich, Garching, Germany
- K. Yoshizawa, K. Ikezoe, Y. Tasaki, D. Kramer, E. Lehmann, G. Scherer
Analysis of gas diffusion layer and flow field design using neutron radiography
 Proc 210th Meeting of the Electrochemical Society, Oct 29- Nov 3, 2006, Cancun, Mexico.
- W. Wagner, P. Allenspach, K. N. Clausen, Y. Dai, H. Glasbrenner, G. Kuehne, H. M. Ronnow, K. Thomsen, G. Zsigmond
SINQ, balancing user operation, development projects ans spin-off support
 Proc. ICANS-XVII, Santa Fe NM, USA, LA-UR-06-3904, 102 (2006)

L. Zanini

Calculation of activation of the MEGAPIE liquid metal target

Radiation Protection and shielding Division conference Carlsbad, April 2-6, 2006.

LECTURES AND COURSES

PD Dr. K. Conder
Keramik II (Semesterprogramm 327-0603-00), Fakultät Werkstoffe ETH Zürich, (zusammen mit Prof. L. Gauckler)

Prof. Dr. H. Grimmer
Kristallographie für Physiker, Universität Zürich, WS 2005/2006

J. Chang
Assistant on the neutron scattering I+II course at ETHZ

H. Heyck
Nuclear Power Generation
University of Applied Science North West Switzerland, SS 2006

H. Heyck
Geschichte der Kernenergie
Reaktorschule PSI, Technikerschule TS

M. Kenzelmann
Magnetism is Strongly Correlated Matter
ETH Zurich, WS 05/06

J. Mesot
Neutronenstreuung in der Festkörperphysik I
ETH Zürich, WS 2005/2006

J. Mesot
Neutronenstreuung in der Festkörperphysik II
ETH Zürich, SS 2006

J. Mesot
ETH Zürich, Seminars WS 2006/2006

J. Mesot
ETH Zürich, Seminars SS 2006

E. Morenzoni,
ETH Zürich, SS-2006
Physik mit Myonen: von der Atomphysik zur Festkörperphysik, Vorlesungen und Übungen

E. Morenzoni,
ETH Zürich, SS-2006
Praktikum: Myon Spin Rotationspektroskopie

V. Pomjakushin
Assistant VP ETHZ, SS+WS

H.M. Rønnow
Assisant VP ETHZ, SS+WS

R. Scheuermann,
Introduction to Muon Spin Rotation (μ SR): Part II: Muonium and Muoniated Radicals,
5th PSI Summer School on Condensed Matter Research,
August 19 – 26, 2006, Zuz, Switzerland

B. Thielemann
Assistant lecture Physik-II, ETHZ

J.A. Paturski
Thermographische Temperaturmessung, Paul Scherrer Institute Lehrkurs

T. Prokscha,
Introduction to Muon Spin Rotation (μ SR): Part I: Basics and Applications,
5th PSI Summer School on Condensed Matter Research,
August 19 – 26, 2006, Zuz, Switzerland

MEMBERSHIP IN EXTERNAL COMMITTEES

A. Amato

- Swiss Representative COST – Action P16, "Emergent Behaviour in Correlated Matter"

D. Herlach,

- Secretary PSI μ SR Research Committee

Dr. K. Clausen

- Member of the ESS-Scandinavia Science Group (since 2004)
- Member of the Board of NMI3 (since 2004)
- Member of the Scientific Selection Panel of the Berlin Neutron Scattering Centre (since 2005)
- Member of the Science Program Advisory Council for Condensed Matter Physics and Nanoelectronics at Research Centre Jülich, Germany (since 2006)
- Chairman of the BENSC Instrument Committee (since 2006)

Dr. P. Allenspach

- Chairman of the European Neutron Scattering Association (ENSA): (since 2006)
- President of the Swiss Neutron Scattering Society (SGN/SSDN): (since 2004)
- Chairman of the ILL subcommittee 7 (2004-2006)
- Member of the Committee of Experts of the NMI3 Networking Activities (since 2004)

Dr. H. Grimmer

- Commission on Mathematical and Theoretical Crystallography of the International Union of Crystallography (since 2005)

Dr. M. Könnecke

- NeXus International Advisory Committee seit 2004
- NOBUGS International Advisory Committee seit 2002 (Chairman, 2006)
- Member of the Data Acquisition and Control Systems Support Group, PSI (since 2003)

Dr. M. Medarde

- 1-External evaluator for the US Department of State for the Science Centers , USA. Since October 2004
- External evaluator for the Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR), Generalitat de Catalunya, Spain. Since March 2005
- Member of the College 5b of the Institut Laue Langevin in Grenoble, France since May 2006

Prof. Dr. A. Furrer

- Forum of the NCCR Network on Materials with Novel Electronic Properties (MaNEP), member (since 2001)
- International Advisory Board of the Centre of Competence in Nanoscience and Advanced Materials (Jagiellonian University, Cracow, Poland), member (since 2002)
- Science Advisory Committee of the EU Neutron/Muon Integrated Infrastructure Initiative (NMI3), member (since 2002)
- Third World Academy of Sciences (TWAS) of the Abdus Salam International Centre for Theoretical Physics (ICTP, Trieste), advisor (since 2003)
- Sonderforschungsbereich 463 der Deutschen Forschungsgemeinschaft (DFG) über "Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport, Dresden", Gutachter (since 2005)
- Large Neutron Infrastructures Expert Group of the European Strategy Forum on Research Infrastructures (ESFRI), member (since 2005)
- International Advisory Committee of the International Conference on Neutron and X-Ray Scattering (ICNX 2007, Indonesia), member (since 2006)

Dr. T. Gutberlet

- International Scientific Advisory Committee, Budapest Neutron Centre, KFKI, since Oct. 2005 ongoing

Prof. M. Kenzelmann

- Referee Board, Physics Review Journals
- Referee Board, NIST Center for Neutron Research

Dr. J. Mesot

- Subcommittee "Structural and Magnetic Excitations" of the Scientific Council, Institute Laue Langevin, Grenoble, France (2000-2006).
- Forum of the CH-NCCR/NSF Materials with Novel Electronic Properties (MaNEP) (since 2005)
- Scientific Committee of FRM2, Munich, DE (since 2005)
- Editor of Neutron News (since 2003).
- Summer School on Condensed Matter Research, yearly, Zuoz, CH: organizing committee (since 2005).
- Conference on Dynamical Properties of Solids (DYPROSO): International Advisory Committee (since 2002).
- Sixth International Workshop on Polarized Neutrons in Condensed Matter Investigations (PNMI 2006), September 25 - 28, 2006, Berlin, DE: International Advisory Committee (since 2005).
- 3rd workshop on Inelastic Neutron Spectrometers 2006 (WINS 2006), September 29-30, 2006, Berlin, DE: International Advisory Board (since 2006).
- 5th International Conference Stripes 2006, December 17-22, 2006, Roma, IT: Scientific Committee.

Dr. B. Roessli

- muSR scientific committee, PSI, member, since 2002
- College 4 committee, ILL, member, since 2006

H. Heyck

- JPARC Materials and Life Science Facility Technical Advisory Committee (N-TAC) JAEA Tokai 2006
- DOE Review Team for the Basic Energy Science Lujan Neutron Scattering Center Los Alamos National Laboratory 2006
- DOE Review Team for the Basic Energy Science Intense Pulsed Neutron Source Argonne National Laboratory 2006

R. Scheuermann

- Membership in internal/external committees
- DACSY (PSI)
- ISMS Facility Subcommittee (until 06.10.2006)
- ISIS Facility Access Panel

H. Van Swygenhoven

- Meeting Chair of the MRS Fall meeting 2006, Boston, USA (6000 attendants, 42 symposia). Co-chairs are Dr. L.J. Terminello (Lawrence Livermore National Laboratory), Dr. B. Chalamala (MCNC Research & Development Institute).
- Member of the Editorial Advisory Panel of the journal "Materials Today", Elsevier, Dec. 2006
- Expert in computational materials science for the EU for the contacts with India and China.

AWARDS

D. Andreica,
μSR under pressure: the method
ICM satellite workshop "Novel pressure-induced phenomena in condensed matter systems"
Best Poster Award, August 26-29, 2006, Fukuoka, Japan

Stefan Brandstetter
Best Poster Award, 14th International Conference of Materials Strength, 4-9.6.2006, Xi'an,
P.R.China

Andreas Elsener
Willi-Studer-Preis für die beste Diplomprüfung im Studiengang Rechnergestützte Wissenschaften
2006, ETH Zürich
SCS Poster Prize, Fallmeeting of the Swiss Chemical Society, October 13th, 2006, Zürich

L. Zanini
Best paper nomination:
Calculation of activation of the MEGAPIE liquid metal target
Radiation Protection and shielding Division conference Carlsbad, April 2-6, 2006.

LIST OF PUBLICATIONS

BIOMOLECULAR RESEARCH

TEACHING ACTIVITIES (LECTURES)

K. Ballmer-Hofer

Molecular virology

University of Basel, CH, WS 2005/2006

K. Ballmer-Hofer

Cell signaling

University of Basel, CH, WS 2006/2007

R. Jaussi

"Molekulare Zellbiologie" für Biochemie- und Biologie-Studierende

University of Zurich, WS 2005/2006

R. Jaussi

„Gentechnik“ für Medizinstudierende

University of Zurich, SS2006

R. Jaussi

Masterkurs in Gentechnik

Einwöchiger Kurs am PSI

University of Zurich

D. Kostrewa

Tutorial course: "Solving ligand-target structure for understanding pharmacology at molecular level"

University of Geneva, CH, SS 2006

F.K. Winkler

Molecular Biology and Biophysics III: Proteins: Structure, Function and Engineering

ETH Zurich, WS 2005/2006

F.K. Winkler

Grundlagen der Biologie I

ETH Zurich, SS 2006

PUBLICATIONS

- F. Brem, L. Tiefenauer, A. Fink, J. Dobson, A.M. Hirt
A mixture of ferritin and magnetite nanoparticles mimics magnetic properties of human brain tissue
Phys. Rev. B 73 (22), 224427-1 – 224427-6 (2006)
- S. Cébe-Suarez, M. Pieren, L. Cariolato, S. Arn, U. Hoffmann, A. Bogucki, C. Manlius., J. Wood, K. Ballmer-Hofer
A VEGF-A splice variant defective for heparan sulfate and neuropilin-1 binding shows attenuated signaling through VEGFR-2
Cell. Mol. Life Sci. 63 (17), 2067-2077 (2006)
- S. Cébe-Suarez, A. Zehnder-Fjallman, K. Ballmer-Hofer
The role of VEGF receptors in angiogenesis; complex partnerships
Cell. Mol. Life Sci. 63 (5), 601-615 (2006)
- S. Honnappa, W. Jahnke, J. Seelig, M.O. Steinmetz
Control of intrinsically disordered stathmin by multisite phosphorylation
J. Biol. Chem. 281 (23), 16078-16083 (2006)
- S. Honnappa, O. Okhrimenko, R. Jaussi, H. Jawhari, I. Jelesarov, F.K. Winkler, M.O. Steinmetz
Key interaction modes of dynamic +TIP networks
Mol. Cell 23 (5), 663-671 (2006)
- A. Javelle, D. Lupo, L. Zheng, X.D. Li, F.K. Winkler, M. Merrick
An unusual twin-His arrangement in the pore of ammonia channels is essential for substrate conductance
J. Biol. Chem. 281 (51), 39492-39498 (2006)
- R.A. Kammerer, M.O. Steinmetz
De novo design of a two-stranded coiled-coil switch peptide
J. Struct. Biol. 155 (2), 146-153 (2006)
- X.D. Li, D. Lupo, L. Zheng, F. Winkler
Structural and functional insights into the AmtB/Mep/Rh protein family.
Transfus. Clin. Biol. 13 (1-2), 65-69 (2006)
- J. Liu, L. Tiefenauer, S. Tian, P.E. Nielsen, W. Knoll
PNA-DNA hybridization study using labeled streptavidin by voltammetry and surface plasmon fluorescence spectroscopy
Anal. Chem. 78 (2), 470-476 (2006)
- P.R. Macdonald, P. Progiás, B. Ciani, S. Patel, U. Mayer, M.O. Steinmetz, R.A. Kammerer
Structure of the extracellular domain of Tie receptor tyrosine kinases and localization of the angiopoietin-binding epitope
J. Biol. Chem. 281 (38), 28408-28414 (2006)
- C. Marty, Z. Langer-Machova, S. Sigrist, H. Schott, R.A. Schwendener, K. Ballmer-Hofer
Isolation and characterization of a scFv antibody specific for tumor endothelial marker 1 (TEM1), a new reagent for targeted tumor therapy
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M. Pieren, A.E. Prota, C. Ruch, D. Kostrewa, A. Wagner, K. Biedermann, F.K. Winkler, K. Ballmer-Hofer
Crystal structure of the Orf virus NZ2 variant of vascular endothelial growth factor-E. Implications for receptor specificity
J. Biol. Chem. 281 (28), 19578-19587 (2006)

A.B. Siemer, C. Ritter, M.O. Steinmetz, M. Ernst, R. Riek, B.H. Meier
¹³C, ¹⁵N Resonance assignment of parts of the HET-s prion protein in its amyloid form
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M.O. Steinmetz
Structure and thermodynamics of the tubulin-stathmin interaction.
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R. Studer, P. Dahinden, W.W. Wang, Y. Auchli, X.D. Li, P. Dimroth
Crystal structure of the carboxyltransferase domain of the oxaloacetate decarboxylase Na⁺ pump from Vibrio cholerae
J. Mol. Biol. in press (2007), available online since 19 December 2006
doi:10.1016/j.jmb.2006.12.035

A. Wagner, M. Pieren, C. Schulze-Briese, K. Ballmer-Hofer, A.E. Prota
Structure determination of VEGF-E by sulfur-SAD
Acta Cryst. D62 (11), 1430-1434 (2006)

F.K. Winkler
Amt/MEP/Rh proteins conduct ammonia
Pflugers Arch. 451 (6), 701-707 (2006)

S.M. Zeisberger, B. Odermatt, C. Marty, A.H. Zehnder-Fjallman, K. Ballmer-Hofer, R.A. Schwendener,
Clodronate-liposome-mediated depletion of tumour-associated macrophages: a new and highly effective antiangiogenic therapy approach
Br. J. Cancer. 95 (3), 272-281 (2006)

CONFERENCE PROCEEDINGS

S. Cébe-Suarez, M. Pieren, L. Cariolato, A. Bogucki, C. Manlius, J. Wood, K. Ballmer-Hofer
VEGF-A splice variant defective for heparan sulfate and neuropilin-1 binding shows attenuated signalling potential through VEGFR-2 (P58)
Targeting the Kinome Conference, Basel, Switzerland, December 4 – 6, 2006

D. Dosch, K. Ballmer-Hofer
The role of dimerisation in VEGFR-2 activation (P59)
Targeting the Kinome Conference, Basel, Switzerland, December 4 – 6, 2006

D. Frey, R. Jaussi, C.Kambach, D. Kostrewa, E. Pohl, A. Prota, C.Schulze-Briese, M.O. Steinmetz, F.K. Winkler
The high throughput cloning & expression screening technology platform at PSI (P 19)
5th International NCCR Symposium on New Trends in Structural Biology, ETH Zurich, Zurich, Switzerland, September 15-16, 2006

S. Honnappa, O. Okhrimenko, R. Jaussi, H. Jawhari, I. Jelesarov, F.K. Winkler, M.O. Steinmetz
Key Interaction modes of dynamic +TIP networks (P17)

5th International NCCR Symposium on New Trends in Structural Biology, ETH Zurich, Zurich, Switzerland, September 15-16, 2006

A. Javelle, D. Lupo, L. Zheng, X.D. Li, M. Merrick, F.K. Winkler

An unusual twin-His arrangement in the pore of ammonia channels is essential for substrate conduction (P 18)

5th International NCCR Symposium on New Trends in Structural Biology, ETH Zurich, Zurich, Switzerland, September 15-16, 2006

D. Lupo, L. Zheng, X.D. Li, F.K. Winkler

Structural analysis of two essential and highly conserved histidine residues of AmtB from E. coli
3rd Int. Conference on Structure, Dynamics and Function of Proteins in Biological Membranes, Monte Verità, Ascona, Switzerland, May 14 – 19, 2006

D. Lupo, M.J. Conroy, A. Durand, X.D. Li, P.A. Bullough, M. Merrick, F.K. Winkler

The crystal structure of the AmtB-GlnK complex (P 20)

5th International NCCR Symposium on New Trends in Structural Biology, ETH Zurich, Zurich, Switzerland, September 15-16, 2006

O. Okhrimenko, S. Honnappa, R. Jaussi, H. Jawhari, F.K. Winkler, M.O. Steinmetz, I. Jelesarov
Thermodynamic analysis of the EB1-p150^{glued} interaction (P 47)

5th International NCCR Symposium on New Trends in Structural Biology, ETH Zurich, Zurich, Switzerland, September 15-16, 2006

M. Pieren, A.E. Prota A. Wagner, D. Kostrewa, F.K. Winkler, K. Biedermann, K. Ballmer-Hofer
Crystal structure of the Orf Virus NZ2 variant of VEGF-E: Implications for VEGF receptor specificity

USGEB, Annual Meeting of the Swiss Societies for Experimental Biology, Geneva, February 23-24, 2006

C. Ruch, A. Prota, M. Steinmetz, G. Skiniotis, T. Walz, K. Ballmer-Hofer

Functional and structural studies of the extracellular ligand binding domain of VEGFR-2
The role of dimerisation in VEGFR-2 activation (P02)

Targeting the Kinome Conference, Basel, Switzerland, December 4 – 6, 2006

M.O. Steinmetz

Key interaction modes of dynamic +TIP networks

46th Annual Meeting of the American Society for Cell Biology, San Diego, USA, December 9-13, 2006

L. Tiefenauer, X. Han, M. DiBerardino

Monitoring mass transport across lipid bilayer membranes using nanopore array chips

9th World Congress of Biosensors, Toronto, Canada, May 10-12, 2006

DISSERTATIONS

M. Pieren

Structure/function analysis of viral vascular endothelial growth factor (VEGF-E) and its specific receptor (VEGFR-2).

ETH Zurich, Diss-ETH Nr. 16571, 31.3.2006

T. Marquardt

Structure-function studies of CRM1-related nuclear transport complexes, the human Obg-like ATPase 1, and the 4-hydroxy-2,3-trans-nonenal reductase AKR11C1 from Bacillus halodurans

ETH Zurich, Diss-ETH Nr. 16659, 31.3.2006

INVITED TALKS

K. Ballmer-Hofer

VEGF signal output is determined by ligand-specific co-receptor ligation

10th Swiss Receptor Workshop, Pharmacenter, Basel, Switzerland, March 12-15, 2006

K. Ballmer-Hofer

Structure of VEGFR-2 extracellular domain in complex with VEGF determined by electron microscopy

Gordon Conference on Growth Factors and Signalling, New London CT, USA, July 16-21, 2006

K. Ballmer-Hofer

What biologists can learn from modern physics

5th PSI Summer School on Condensed Matter Research, Zuz, Switzerland, August 19-26, 2006

K. Ballmer-Hofer

Neue Möglichkeiten einer kombinierten Tumorthherapie basierend auf Angiogeneseinhibitoren und Bisphosphonaten

Claraspital, Basel, Switzerland, October 10, 2006

F. Brem, A.M. Hirt, L. Tiefenauer, H.G. Wieser, J. Dobson

Can a two-component nanoparticle system mimic the magnetic properties of human brain tissue?

6th Int. Conference on "Scientific and clinical of magnetic carriers", Krems, Austria, May 17-20, 2006

X. Han, L. Tiefenauer

Monitoring melittin interaction with free-standing lipid bilayers suspended in nanopores

Int. Workshop on "Dynamics of artificial and biological membranes", Gomadingen, Germany, March 20-22, 2006

X.D. Li

AmtB/Mep/Rh proteins: channels or transporters?

6th D-BIOL Symposium ETH Zurich, Davos, Switzerland, May 24-26, 2006

X.D. Li

Structural and functional insights into the AmtB/Mep/Rh protein family

Int. Conference on Rh protein superfamily, Paris, France, May 3-4, 2006

A.E. Prota

Crystal structure of the Orf virus NZ2 variant of VEGF-E: Implications for receptor Specificity

Dipartimento delle Scienze Farmaceutiche, Università degli Studi di Bologna, Bologna, Italy,
June 26, 2006

M.O. Steinmetz

Control of intrinsically disordered stathmin by multisite phosphorylation

Int. Conference on Structural Analysis of Supramolecular Assemblies by Hybrid Methods, Lake
Tahoe, CA, USA, March 15-19, 2006

M.O. Steinmetz

Tales of molecular mechanisms: From actin to tubulin

Ueli Aebi 60th Birthday Symposium, Zentrum Paul Klee, Bern, June 2, 2006

M.O. Steinmetz

Key interaction modes of dynamic +TIP networks

21st European Cytoskeleton Forum, Biopolis, Singapore, October 31 - November 4, 2006

A. Studer, F.K. Winkler, L. Tiefenauer

Functional assays for membrane proteins using nanopore array chips

Int. Workshop on "Dynamics of artificial and biological membranes", Gomadingen, Germany,
March 20-22, 2006.

L. Tiefenauer

Nanopore arrays for investigating transmembrane processes

Seminar at ETH Zürich, Lab. of Biosensors and Bioelectronics, December 1, 2006

L. Tiefenauer

Nanotechnology and societal acceptance

Nanoconvention 06, Bern, Switzerland. June 23, 2006

L. Tiefenauer

Nanopore arrays for investigating transmembrane processes

Laboratory of Biosensors and Bioelectronics, ETH Zurich, Zurich, December 1, 2006

F.K. Winkler

The pore structure of Amt/Mep/Rh proteins: ammonia versus ammonium conduction

3rd International Conference on Structure, Dynamics and Function of Proteins in Biological
Membranes, Ascona, Switzerland, May 14-19, 2006

F.K. Winkler

Amt/Rh proteins and ammonia

4th Int. Hannover Conference on Hepatic Encephalopathy, Dresden, Germany, June 10-12, 2006

F.K. Winkler

Ammonia channels: mechanism and regulation

Switzerland-Japan Symposium on Structural Biology 2006, Brunnen, Switzerland, September 17-
19, 2006

BOOK CHAPTERS

L.X. Tiefenauer

Magnetic nanoparticles as contrast agents for medical diagnosis

In: "Nanotechnology in biology and medicine", T. Vo-Dinh (ed.), CRC Press, LCC, Chapter 23, p. 413-432 (2006)

CENTER FOR RADIOPHARMACEUTICAL SCIENCE

TEACHING ACTIVITIES (LECTURES)

P.A. Schubiger, S.M. Ametamey, R. Schibli

Radiopharmazeutische Chemie

ETH Zürich WS05/06

P.A. Schubiger, S.M. Ametamey, R. Schibli et. al.

Einführung in die pharmazeutischen Wissenschaften I und II

ETH Zürich WS05/06 und SS06

P.A. Schubiger, R. Schibli, et al.

Drug Discovery Seminars

ETH Zürich, WS05/06

PUBLICATIONS

S.M. Ametamey, L. Kessler, M. Honer, M.T. Wyss, A. Buck, S. Hintermann, Y.P. Auberson, F. Gasparini, P.A. Schubiger

Radiosynthesis and preclinical evaluation of ¹¹C-ABP688 as a probe for imaging the metabotropic glutamate receptor subtype 5 (mGluR5)

J. Nucl. Med. 47, 698-705 (2006)

S.M. Ametamey, P.A. Schubiger

PET pharmaceuticals for neuroreceptor imaging

Nuc. Sci. Technique 17, 139-143 (2006)

J.E. Arlt, I. Novak-Hofer, D. Gast, V. Gschwend, G. Moldenhauer, J. Grünberg, M. Honer,

P.A. Schubiger, P. Altevogt, A. Krüger

Efficient inhibition of i.p. tumor growth and dissemination of human ovarian carcinoma cells in nude mice by anti-L1-cell-adhesion molecule monoclonal antibody treatment

Cancer Res. 66, 936-943 (2006)

- A. Bettio, M. Honer, C. Müller, M. Brühlmeier, U. Müller, R. Schibli, V. Groehn, P.A. Schubiger, S.M. Ametamey
Synthesis and preclinical evaluation of a ^{18}F -labelled folic acid derivative for PET imaging of folate receptor-positive tumours
J. Nucl. Med. 47, 1153-1160 (2006)
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Immunoscintigraphy of patients with head and neck squamous cell carcinomas, with a human anti-angiogenetic antibody fragment
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*Automated no-carrier-added synthesis of $[1-^{11}\text{C}]$ -labeled *d*- and *l*-enantiomers of lactic acid*
Appl. Radiat. Isot. 64 (12), 1613-1622 (2006)
- G. Folkers, A. Ishai, M. Rudin, P.A. Schubiger, M. Bräutigam, H. Möhler, H.P. Märki
Imaging in Biomedical Research
Chimia, 60, 805-814 (2006)
- E. Garcia-Garayoa, V. Maes, P. Bläuenstein, A. Blanc, A. Hohn, D. Tourwé, P.A. Schubiger
Double-stabilized neurotensin analogues as potential radiopharmaceuticals for NTR-positive tumors
Nucl. Med. Biol. 33, 495-503 (2006)
- M. Honer, B. Hengerer, M. Blagoev, S. Hintermann, P. Waldmeier, P.A. Schubiger, S.M. Ametamey
Comparison of $[^{18}\text{F}]\text{FMT}$ and $[^{18}\text{F}]\text{FECNT}$ for imaging dopaminergic neurotransmission in mice
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- A. Johayem, S. Raic, K. Lazzatic, P.A. Schubiger, L. Scapozza, S.M. Ametamey
Synthesis and characterization of a C-6 nucleoside analogue for in vivo imaging of herpes simplex virus type 1 thymidine kinase gene expression via PET
Chem. Biodivers. 3, 274-282 (2006)
- Y.S. Kim, Z.J. Hea, R. Schibli, S. Liu
Synthesis, characterization and X-ray crystal structure of $\text{Re}(\text{L}4)(\text{CO})_3 \text{Br} \cdot 2\text{CH}_3\text{OH}$ ($\text{L}4 = \text{N}, \text{N}$ -bis(2-diphenylphosphino)ethyl-methoxyethylamine): A model compound for novel cationic $\text{Tc-99m}(\text{I})$ -tricarbonyl radiotracers useful for heart imaging
Inorg. Chim. Acta 359, 2479 (2006)
- K. Knogler, J. Grünberg, I. Novak-Hofer, K. Zimmermann, P.A. Schubiger
Evaluation of ^{177}Lu -DOTA labeled aglycosylated monoclonal anti-L1-CAM antibody chCE7: Influence of the number of chelators on the in vitro and in vivo properties
Nucl. Med. Biol. 33, 883-889 (2006)
- S. Kubetzko, E. Balic, R. Waibel, U. Zangenmeister-Wittke, A. Plückthun
Pegylation and multimerization of the anti-P185^{Her-2} single-chain FV fragment 4D5: Effect on tumor targeting
J. Biol. Chem 281, 35186-35201(2006)
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Water-exchange study revealed unexpected substitution behavior of $[(\text{CO})_2(\text{NO})\text{Re}(\text{H}_2\text{O})_3]^{2+}$ in aqueous media
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Novel ^{99m}Tc labeled neurotensin analogues with optimized biodistribution properties
J. Med. Chem. 49, 1833-1836 (2006)
- C.M. Matter, M.T. Wyss, P. Meier, N. Spath, T. von Lukowicz, C. Lohmann, B. Weber, A.R. de Molina, J.C. Lacal, S.M. Ametamey, G.K. von Schulthess, T.F. Luscher, P.A. Kaufmann, A. Buck
¹⁸F-cholin images murine atherosclerotic plaques ex vivo
Arterioscler. Thromb. Vasc. Biol. 26, 584-589 (2006)
- T.L. Mindt, H. Struthers, L. Brans, T. Anguelov, C. Schweinsberg, V. Maes, D. Tourwe, R. Schibli
"Click to chelate": Synthesis and installation of metal chelates into biomolecules in a single step
J. Am. Chem. Soc. 128; 15096 (2006)
- L. Mu, K. Drandarov, W.H. Bisson, A. Schibig, C. Wirz, P.A. Schubiger, G. Westera
Synthesis and binding studies of epibatidine analogues as ligands for nicotinic acetylcholin receptors
Eur. J. Med. Chem. 41, 640-650 (2006)
- C. Müller, P.A. Schubiger, R. Schibli
Synthesis and in vitro/in vivo evaluation of novel ^{99m}Tc(CO)₃-follates
Bioconjug. Chem. 17, 797-806 (2006)
- C. Müller, M. Brühlmeier, P.A. Schubiger, R. Schibli
Effects of antifolate drugs on the cellular uptake of radiofolates In vitro and In vivo
J. Nucl. Med. 47, 2057 (2006)
- C. Müller, A. Hohn, P.A. Schubiger, R. Schibli
Preclinical evaluation of novel organometallic ^{99m}Tc-folate and ^{99m}Tc-pterolate radiotracers for folate receptor-positive tumor targeting
Eur. J. Nucl. Med. 33, 1007 (2006)
- C. Müller, P.A. Schubiger, R. Schibli
In vitro and in vivo targeting of different folate receptor-positive cancer cell lines with a novel ^{99m}Tc-radiofolate tracer
Eur. J. Nucl. Med. 33, 11620 (2006)
- O. Riesterer, M. Honer, W. Jochum, C. Oehler, S. Ametamey, M. Pruschy
Ionizing radiation antagonizes tumor hypoxia induced by antiangiogenic treatment
Clin. Cancer Res. 12, 3518-3524 (2006)
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Uptake of ¹⁸F-fluorocholin, ¹⁸F-fluoro-ethyl-L-tyrosine and ¹⁸F-fluoro-2-deoxyglucose in F98 gliomas in the rat
Eur. J. Nucl. Med. Mol. Imaging 33, 673-682 (2006)
- M.T. Wyss, M. Honer, P.A. Schubiger, S.M. Ametamey
NanoPET imaging of [¹⁸F]fluoromisonidazole uptake in experimental mouse tumours
Eur. J. Nucl. Med. Mol. Imaging 33, 311-318 (2006)

CONFERENCE PROCEEDINGS

T. Anguelov

Synthesis and In Vitro Evaluation of Novel Tc- and Re-Containing Human Thymidine Kinase 1 Substrates

7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

D. Desbouis

Thymidine derivatives labeled with technetium-99m as reporter probes for suicide gene therapy

3rd International Symposium on Bioorganometallic Chemistry, Milan, Italy, July 5 – 8, 2006

A. Friedli, I. Novak-Hofer, S. Cohrs, P.A. Schubiger, J. Grünberg

Anti L1-CAM antibody chCE7 inhibits proliferation of tumor cells independent of apoptosis

4th Swiss Apoptosis Meeting, University of Bern, Bern, Switzerland, August 24 – 25, 2006,

E. Garcia Garayoa, C. Schweinsberg, D. Rüegg, V. Maes, A. Blanc, P. Bläuenstein, D. Tourwé, P.A. Schubiger

Influence of the spacer on the biodistribution of radiolabelled bombesin analogues

Eur.J.Nucl. Med 33, Suppl. 2, 33, S150 (2006)

E. Garcia Garayoa, C. Schweinsberg, V. Maes, A. Blanc, P. Bläuenstein, D. Tourwé, P.A. Schubiger

Increased in vivo tumor uptake with new stabilized bombesin analogues. Q

J. Nucl. Med. 50, Suppl. 1, 15-16 (2006)

E. Garcia Garayoa, C. Schweinsberg, A. Blanc, P. Bläuenstein

Technetium-99m-tricarbonyl bombesin: preclinical evaluation of new analogues with different spacers

7. Jahreskongress SGNM/SSMN, Lausanne, Switzerland, June 1 – 3, 2006

N.I. Gorshkov

Complexation of the $[M(CO)_2(NO)]^{2+}$ core ($M = Re, 99mTc, 99Tc$) with bidentate and tridentate Ligands

7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

J. Grünberg, K. Knogler, K. Zimmermann, S. Cohrs, P.A. Schubiger, I. Novak-Hofer

Comparison of two different Cu-67-labeled chCE7 antibody variants in nude mice bearing human metastatic ovarian carcinoma

Eur.J.Nucl. Med 33, Suppl. 2, 33, S90 (2006)

J. Grünberg., I. Novak-Hofer, K. Knogler, K. Zimmermann, P. Bläuenstein, H.R. Mäcke, P.A. Schubiger

¹⁷⁷Lu- and ⁶⁷Cu-labeled recombinant chCE7F(ab')₂ fragments for targeting of L1-CAM positive tumors.

7. Jahreskongress SGNM/SSMN, Lausanne, Switzerland, June 1 – 3, 2006

A. Hohn

Production of nca ¹⁸⁶Re from highly enriched ¹⁸⁶W at a cyclotron,

7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

M. Honer, T. Ebenhan, P. McSheehy, P.A. Schubiger, S.M. Ametamey
Comparison of ¹⁸F-FDG, 3'-deoxy-3'-¹⁸F-fluorothymidine, ¹⁸F-fluorocholine and ¹⁸F-fluoro-L-tyrosine uptake in various murine and rat tumor models measured by high-resolution PET'
5th Annual Meeting of the Society of Molecular Imaging, Waikoloa Village, Big Island of Hawaii, August 30 – September 2, 2006

T.L. Mindt
Amino acid-specific modification of proteins for diagnostic and therapeutic purposes using transglutaminases
232nd National Meeting of the American Chemical Society, San Francisco, USA, September 10 - 14, 2006

S. Jeger
Development of novel enzymatic methods for amino acid-specific modification of diagnostic and therapeutic proteins
7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

M. Lyczko
Exchange of the water molecule in aqua N-methyl-2-pyridinecarbothioamide tricarbonyl technetium(I) cation for imidazol and bombesin. 2+1 approach
7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

T.L. Mindt
"Click to chelate": simultaneous synthesis and introduction of polydentate metal chelators into biomolecules for radiopharmaceutical applications
232nd National Meeting of the American Chemical Society, San Francisco, USA, September 10 - 14, 2006

T.L. Mindt
Amino acid-specific modification of proteins for diagnostic and therapeutic purposes using transglutaminases
232nd National Meeting of the American Chemical Society, San Francisco, USA, September 10 - 14, 2006

C. Müller
In vivo comparison of ^{99m}Tc- and ¹⁸⁸Re-labeled radiofolates for potential use in diagnostic and therapeutic nuclear medicine
7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

C. Müller
Antifolates significantly reduce undesired kidney accumulation of tumor targeting radiofolates
19th Annual Meeting of the European Association of Nuclear Medicine, Athens, Greece, September 30 – October 4, 2006

I. Novak-Hofer, K. Knogler, J. Grünberg, K. Zimmermann, S. Cohrs, M. Honer, P. Altevogt, P.A. Schubiger
L1-Targeted Cu-67-radioimmunotherapy in combination with immunotherapy for treatment of ovarian cancer metastases
53rd Annual Meeting of the American Society of Nuclear Medicine, San Diego, USA, June 3 – 7, 2006

R. Schibli
Preclinical SPECT/CT analyses of radiofolates combined with chemotherapeutics
European Society of Molecular Imaging, Paris, France, May 17 – 19, 2006,

R. Schibli
Design of polydentate triazole metal chelates via "click" chemistry
37th International Conference of Coordination Chemistry, Cape Town, South Africa, August 13 – 18, 2006

H. Struthers
Investigating the substitution behavior of mixed carbonyl-nitrosyl precursors of rhenium and technetium in the presence of tetradentate ligands
7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone, Italy, September 6 – 9, 2006

DISSERTATIONS

K. Knogler
Comparison of different radiometal-labeled antibody formats for imaging and therapy of L1-CAM positive tumors
ETH Zürich, Nr. 16587, April 2006

INVITED TALKS

S.M. Ametamey
PET Radiopharmaceuticals for monitoring therapy
27th International Symposium on Radioactive Isotopes in Clinical Medical Research, Bad Gastein, Austria, January 11 – 14, 2006

S.M. Ametamey
PET radiopharmaceuticals: From development to human studies
Symposium zu Ehren von Prof. Heimgartner, ETHZ, Zürich, Switzerland, June 9, 2006

S.M. Ametamey
Functional Imaging with PET,
Polyphor, Basel, Switzerland, October 19, 2006

S.M. Ametamey
Positron emission tomography in small laboratory animals
Workshop on New Techniques in Lab Animal Science, Fribourg, Switzerland, November 21 – 22, 2006,

P. Bläuenstein

New therapeutic radioisotopes, continuing medical education

19th Annual Meeting of the European Association of Nuclear Medicine, Athens, Greece,
September 30 – October 4, 2006

J. Grünberg

Das L1 Zelladhäsions-Molekül (L1-CAM): Ein potenzielles Target für Radioimmuntherapie

Institut für Biochemie und Lebensmittelchemie, Universität Hamburg, Germany, January 16, 2006

J. Grünberg, I. Novak-Hofer

Production of recombinant antibody formats in HEK293 cells

University Hospital Zürich, Oncology Dept., Zürich, December 19, 2006

M. Honer

Application of small animal PET in research and preclinical development,

Philipps Research Laboratories, Eindhoven, The Netherlands, November 17, 2006,

M. Martic

Synthesis of C-6 pyrimidine derivatives as potential thymidine kinase substrates

Jahrestreffen der Schweizerischen Gesellschaft für Radiologie, Lausanne, Switzerland, June 2,
2006

I. Novak-Hofer

L1-CAM as Target for tumor imaging and therapy

Proteomics Center, ETHZ, Zürich, Switzerland, June 16, 2006

I. Novak-Hofer

⁶⁷Cu-radioimmunotherapy and growth inhibition by anti-L1 antibodies in a therapy model of ovarian cancer metastasis

Deutsches Krebsforschungszentrum Heidelberg, Abteilung Zelluläre Immunologie, Heidelberg,
Germany, November 23, 2006

I. Novak-Hofer, J. Grünberg

Radioimmunotherapy and radioimmunodiagnosis of L1-CAM expressing tumors

University Hospital Zürich, Oncology Dept., Zürich, December 19, 2006

R. Schibli

Organometallic radiolabeling cores for diagnosis and therapy: Nice to have or need to have?

Seminars at the Inorganic Department of the Free University of Berlin, Germany, February 2006

R. Schibli

Amino acid-specific modification of proteins for diagnostic and therapeutic purposes using transglutaminases

23rd International Conference Advances in the Application of Monoclonal Antibodies in Clinical
Oncology, Mykonos, Greece, June 26 – 28, 2006

R. Schibli

*Organometallic Precursors of Technetium and Rhenium: Unique Opportunities for Radiotracer
Development Due to Chemical Diversity,*

7th International Symposium on Technetium in Chemistry and Nuclear Medicine, Bressanone,
Italy, September 6 – 9, 2006

R. Schibli

Radiopharmaceuticals: From Immuno-PET to Radioimmunotherapy,
19th Annual Meeting of the European Association of Nuclear Medicine, Athens, Greece,
September 30 – October 4, 2006

R. Schibli

Radioactive "Trojan horses": A promising concept in diagnosis and therapy of cancer
Seminare in den Grenzgebieten der Nuklearmedizin, Basel, Switzerland, October 15, 2006,

R. Schibli

Organometallic radiolabeling cores for SPECT and therapy: Nice to have or need to have?
9th Congress of the World Federation of Nuclear Medicine and Biology, Seoul, South Korea,
October 22 – 27, 2006

P.A. Schubiger

Krankhafte Vorgänge sichtbar machen
Senioren Kolleg Liechtenstein, Mauren, Liechtenstein, April 27, 2006

P.A. Schubiger

Molecular imaging with PET tracers and animal PET scanner
Mini Symposium "Imaging in Biomedical Research" University Basel, Switzerland, May 18, 2006

P.A. Schubiger

Radiopharmazeutika zur Diagnose und Therapie von Krankheiten
Reha-Klinik Bad Zurzach, Switzerland, September 21, 2006

P.A. Schubiger

PET in research and development
19th Annual Meeting of the European Association of Nuclear Medicine, Athens, Greece,
September 30 – October 4, 2006

BOOK CHAPTERS

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Lomax A.J., Jäkel O.
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Timmermann B.
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PTCOG 44, PSI Village, June 2006.

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The variability of respiratory liver motion and it's influence on gating accuracy

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Mueller B., Lomax A.J.
Lehrauftrag *Physics in Medial Research*
Winter Semester 2006-07, D-PHYS, ETH, Zurich.

Timmermann B.
Vorlesung *Protonentherapie*
Gegeben im WS 2005/2006, SS 2006, WS 2006/2007 für den Studentenunterricht an der Universität
Münster/Deutschland, Fachbereich Strahlentherapie

MEMBERSHIP IN EXTERNAL COMMITTEES

Lomax A.J.
- Scientific committee for the biennial ESTRO Physics meeting, Barcelona, September 2007
- Member of the International Advisory Board for 'Physics in Medicine and Biology'
- Chairman of the SBMP (Swiss professional body for medical physics) ad-hoc task-group for medical physics training of radiation oncology residents.
- SASRO (Swiss Association of Scientific Radiation Oncology) Board member.
- Chairman of the scientific committee (Physics) for SASRO congress 2006.
Consultant to the IAEA on report IAEA(NDS)-0504 "Nuclear data of Charged-Particle Interactions for Medical Therapy Applications".

E. Pedroni:
membership in the Program Advisory Committee, Biophysics & Radio-Biology, Gesellschaft für
Schwerionenforschung mbH, Planckstr.1, 64291 Darmstadt

Timmermann B.
- German Society for Radiation Oncology (DEGRO)
- German Society for Pediatric Oncology and Hematology (GPOH)
- German Working Group for Pediatric Radio-Oncology (APRO)
- International Society for Pediatric Oncology (SIOP)
- Swiss Working Group for Radio-Oncology (SASRO)
- German Cancer League (DKG)
- Swiss Pediatric Oncology Group (SPOG)
- Member of the German Childhood Brain Tumour Committee (HIT)
- Member of the European Childhood Brain Tumour Sub-Committee (SIOP-BTC)

AWARDS

Bolsi A.
Best poster Award 2006 *Daily patient positioning protocol compared with NAL and SAL protocols*
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Einführung in die Human Reliability Analysis,
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"Comportement des radionuclides dans l'environnement",

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Centre universitaire d'étude des problèmes de l'énergie, University of Geneva, Geneva, Switzerland, Winter Semester 2006

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"Strategische Übung: Kernbrennstoffe", "Analytische Chemie V"

ETH, Zurich, Switzerland, Winter Semester 2006

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"Life Cycle Analysis and other Approaches for Sustainability Assessment"

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Doctoral School, EPFL, Lausanne, Switzerland, Summer Semester 2006

JANSSENS K.

"Cellular Automata for Microstructure Evolution Modeling"

Computational Micro- and Nano-Structures, ETHZ, Zurich, Switzerland, 14-28 June 2006

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"Radioisotope and Radiation Applications"

EPFL doctoral course, PSI, Villigen, Switzerland, Winter Semester 2006

MACIAN-JUAN R.

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Publications in Books

ABOLHASSANI-DADRAS S., RESTANI R., REBAC T., GRÖSCHEL F., HOFFELNER W., BART G., GOLL W.¹, AESCHBACH F.²

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in Peter Rudling, Bruce Kammenzind (Eds): TEM examinations of the metal-oxide interface of zirconium-based alloys irradiated in a pressurised water reactor, ASTM, West Conshohocken, USA, 467-493, 2006 (ISBN JAI12390)

¹ AREVA NP GmbH, Erlangen, DE

² KKG, Däniken, CH

AKSAN S.N.

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BRADBURY M.H., BAEYENS B.

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¹ EMPA, Dübendorf, CH

ARIMA T.¹, YAMASAKI S.¹, YAMAHIRA K.¹, IDEMITSU K.¹, INAGAKI Y.¹, DEGUELDRE C.

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¹ University of Kyushu, Fukuoka, JP

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BONHOUR E.¹, BAUR I.², WIELAND E., JOHNSON C.³, SCHEIDEGGER A.M.

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¹ LURE, Paris, FR

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¹ FZJ, Jülich, DE

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CHEN J.C., HE Z.¹, JUNG P.¹

"Microstructure of helium-implanted α -Al₂O₃ after annealing"

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¹ Université de Strasbourg, Strasbourg, FR

- DÄHN R., JULLIEN M.¹, SCHEIDEGGER A.M., POINSSOT C.¹, BAEYENS B., BRADBURY M.H.
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¹ CEA, Gif-sur-Yvette, FR
- DEGUELDRE C., GUÉNEAU C.¹
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¹ CEA, Gif-sur-Yvette, FR
- DEGUELDRE C., AMATO A., BART G.
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"Feeling defects in zircaloy by extended X-ray absorption fine structure and muon spin relaxation analyses"
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¹ LANL, Los Alamos, US
- DEGUELDRE C., GOMÉZ-BRICENDO D.¹, FANGHÄNEL T.², WARIN D.³
"Editorial Note"
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¹ CIEMAT, Madrid, ES
² FZK, Karlsruhe, DE
³ CEA, Gif-sur-Yvette, FR
- DEGUELDRE C., SCHRAMM R.¹
"IMF Editorial Note"
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¹ NRG, Petten, NL
- DEGUELDRE C., FAVARGER P.¹, ROSSÉ R., WOLD S.²
"Gold colloid analysis by inductively coupled plasma — mass spectrometry in a single particle mode"
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¹ NRG, Petten, NL
² CEA, Cadarache, FR
³ Nexia Solution Ltd, Preston, US
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¹ University of Neuchâtel, Neuchâtel, CH
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¹ AREVA NP GmbH, Erlangen, DE
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¹ AREVA NP GmbH, Erlangen, DE

HASTE T., HERRANZ L.¹, MICAELLI J.²

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¹ CIEMAT, Madrid, ES

² IRSN, St Paul lez Durance, FR

HASTE T., BIRCHLEY J., CAZZOLI E.¹, VITÁZKOVA J.¹

"MELCOR Simulation of the TMI-2 Severe Accident and Initial Recovery Phases"

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¹ Cazzoli Consulting, Nussbaumen, CH

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"Sustainability of current electricity supply technologies: a comparative evaluation"

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HORVATH M.I., GUILLONG M., HELLWIG C., GÜNTHER-LEOPOLD I., IZMER A., KIVEL N., RESTANI R., GÜNTHER D.¹

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¹ ETHZ, Zurich, CH

HORVATH M.I., WIEDMER S.¹, SPINNER T.¹, LUNDMARK R.J.², LONER H.²

"Climate policy and nuclear energy (new clear energy)"

Int. Young Nuclear Congress (IYNC) 2006, IYNC, Stockholm, Sweden, 18-23 June 2006, CD-ROM, 2006

¹ KKG, Däniken, CH

² KKL, Leibstadt, CH

JASIULEVICIUS A., MACIAN-JUAN R.

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LEBRAT J.F.¹, PLASCHY M., TOMMASI J.¹, SUTEAU C.¹, PLISSON-RIEUNDIR D.¹, DE SAINT JEAN C.¹
“Comparative Analysis of Selected Aspects of the MUSE-4 Experiments with the JEF-2.2 and JEFF-3.1 Libraries”

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¹ CEA, Cadarache, FR

LEDERGERBER G.¹, KAUFMANN W.¹, MAGNUSON K.A.², GAVILLET D., ABOLHASSANI-DADRAS S.
“Characterization of Magnetic Crud on KKL Fuel Rods”

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¹ KKL, Leibstadt, CH

² Westinghouse Atom AG, Västerås, SE

MICAELLI J.¹, VAN DORSSLAERE J.², CHAUMONT B.³, HASTE T., MEYER L.⁴, BONNET J.M.³, TRAMBAUER K.⁵, BERAHA D.⁵, ANNUNZIATO A.⁶, SEHGAL B.⁷

“Network of excellence for a sustainable integration of European research on severe accident phenomenology (SARNET)”

FISA 2006, EU Research and Training in Reactor Systems, 13-16 March 2006, Luxembourg, Luxembourg, CD-ROM, Vol. EUR 21231, 144-156, 2006 (ISBN 92-79-01214-2)

¹ IRSN, St Paul lez Durance, FR

² IRSN, Cadarache, FR

³ CEA, Cadarache, FR

⁴ FZK, Karlsruhe, DE

⁵ GRS, Garching, DE

⁶ EC-JRC/ISIS, Ispra, IT

⁷ KTH, Stockholm, SE

MITCHELL C.¹, POETTE C.², PEERS K.¹, CODDINGTON P., SOMERS J.³, VAN-GOETHEM G.⁴
“GCFR: The European Union's Gas-Cooled Fast Reactor Project”

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¹ NNC, Knutsford, UK

² CEA, Cadarache, FR

³ ITU, Karlsruhe, DE

⁴ EC, Brussels, BE

MITCHELL C.¹, MCDERMOTT M.¹, PEERS K.¹, POETTE C.², CODDINGTON P., SOMERS J.³
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¹ NNC, Knutsford, UK

² CEA, Cadarache, FR

³ ITU, Karlsruhe, DE

MORIWAKI M.¹, DONES R., FESENKO S.¹, FALCK W.², OMOTO A.¹
“Development of INPRO Methodology in the Area of Environment”

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¹ IAEA, Vienna, AT

² Consultant, Erlangen, DE

- MURPHY M., PLASCHY M., JATUFF F., BERGMANN U.¹, CHAWLA R.
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 ECCOMAS CFD 2006, 5-8 September 2006, Egmond aan Zee, Netherlands, CD-ROM, 2006 (ISBN 90-9020970-0)
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- PLASCHY M., MURPHY M., JATUFF F., SEILER R., CHAWLA R.
"Experimental Critical Loading and Control Rod Worths in LWR-PROTEUS Configurations Compared with MCNPX Results"
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"Microstructure and hardness properties of irradiated γ -TiAl"
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- ¹ FZJ, Jülich, DE
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"A Technique for Scaling of Decision Error Opportunities Based on Situational Features Identified from Operational Events"
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- REER B.
"Situationsbezogene Faktoren bei der Entstehung von Fehlentscheidungen"
 Menschliche Zuverlässigkeit, 5-6 October 2006, Munich, Germany, CD-ROM, 2006
- RITTER S., SEIFERT H.P.
"Effect of Corrosion Potential on the Corrosion Fatigue Crack Growth Behaviour of Low-Alloy Steels in High-Temperature Water"
 EUROCORR 2006, 24-28 September 2006, Maastricht, Netherlands, CD-ROM, 2006

SCHULENBERG T.¹, STARFLINGER J.¹, AKSAN S.N., BITTERMANN D.², HEIKINHEIMO L.³
“Supercritical water reactor research in the GIF context: current status and future prospects with emphasis on European activities”

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¹ FZK, Karlsruhe, DE

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³ VTT Energy, Espoo, FI

SEIFERT H.P., RITTER S.

“Effect of the Electrochemical Corrosion Potential on the Corrosion Fatigue Crack Growth Behaviour of Low-Alloy Steels in High-Temperature Water”

Annual Meeting of the International Co-operative Group on Environmentally-Assisted Cracking of Water Reactor Materials, 14-19 May 2006, Charleston, SC, USA, CD-ROM, 2006

SWAILES D.¹, AMMAR Y., REEKS M.¹

“Simulation of the Agglomeration and Breakup of Agglomerates in a Random Symmetric Shear Flow”

7th International Aerosol Conference, 10-15 September 2006, St. Paul, USA, CD-ROM, 2006 (ISBN 978-09788735-0-9)

¹ University of Newcastle, GB

VASILIEV A., KOLBE E., ZIMMERMANN M.A.

“Assessment of Standard Point-Wise Neutron Data Libraries for Criticality Safety Analysis with a Monte Carlo Code”

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VASILIEV A., FERROUKHI H., ZIMMERMANN M.A.

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PHYSOR-2006, 10-14 September 2006, Vancouver, Canada, CD-ROM, 2006 (ISBN 0-89448-697-7)

¹ CERN, Geneva, CH

ZBORAY R., PALADINO D., AUBAN O.

“Experiments on Gas Mixing and Stratification Driven by Jets and Plumes in Large-Scale, Multi-Compartment Geometries”

14th Int. Conference on Nuclear Engineering (ICONE14), 17-20 July 2006, Miami, USA, CD-ROM, 2006 (ISBN 0-7918-3783-1)

ZIO E.¹, PODOFILLINI L.

“Exploiting Importance Measures Information For Optimizing System Design By Genetic Algorithms”

2006 European Safety and Reliability Conference (ESREL 2006), 18-22 September 2006, Estoril, Portugal, Vol. 1, 661-669, 2006

¹ Polytechnic of Milan, Milan, IT

Talks delivered at Conferences, Workshops and Specialist Meetings (without Proceedings)

ABOLHASSANI-DADRAS S.

"Recent examinations by TEM on FIB samples prepared from metal-oxide layers"
FIB USER GROUP EMPA, Invited Talk, EMPA, Dübendorf, Switzerland, 27 October 2006

AKSAN S.N.

"Current Status on R&D Activities in Europe for the High Performance Light Water Reactor: Safety and Heat Transfer"

Code Application and Maintenance Programme (CAMP) Meeting, CD-ROM, Invited Talk, NRC, Linthicum, USA, 26-27 October 2006

AKSAN S.N.

"Current Status of R&D Activities in Europe for the High Performance Light Water Reactor: Safety and Heat Transfer"

IAEA Consultancy Meeting on "Heat Transfer Behaviour and Thermo-Hydraulics Code Testing for SCWRs", CD-ROM, Invited Talk, IAEA, Vienna, Austria, 25-26 May 2006

ANDREANI M.

"Basic Validation of CFD Codes for Containment Thermal-Hydraulics"

Seminar at the Division of Nuclear Power Safety, Invited Talk, KTH, Stockholm, Sweden, 27 April 2006

BAKO B., WEYGAND D.¹, SAMARAS M., CHEN J.C., POUCHON M.A., GUMBSCH P.¹

"DDD Simulations of Interactions between Y₂O₃ Oxide Particles and an Edge Dislocation in ODS Materials"

Fall MRS 2006, CD-ROM, MRS, Boston, USA, 27 November - 1 December 2006

¹ IZBS University of Karlsruhe, Karlsruhe, DE

BARTEN W., JASIULEVICIUS A., ZERKAK O., MACIAN-JUAN R.

"Calculations of UMSICHT Water Hammer Benchmark (Experiment 329) using TRACE and RELAP5"

CAMP Spring Meeting, Universidad Politecnica de Valencia, Valencia, Spain, 24-26 May 2006

BERTSCH J.

"Bruchmechanik an Zircaloy-Hüllrohren"

SVMT Fachgruppe Strukturintegrität, SVMT, Villigen, Switzerland, 29 March 2006

BERTSCH J., ALAM A., ZUBLER R.

"Validation of zircaloy tube tensile test for J-R curve determination"

E-MRS Spring Meeting 2006, E-MRS, Nice, France, 29 May - 2 June 2006

BURGHERR P., HIRSCHBERG S.

"Severe accidents in the energy sector: a comparative perspective"

Energy Infrastructure Security & Crisis Management IQPC-Oil & Gas IQ, IQPC, London, United Kingdom, 25-26 April 2006

CAVEDON J.M.

"Advanced Fuel Cycles and Waste Management"

OECD NEA, 9th IEM on Actinide and Fission Partitioning and Transmutation, Invited Talk, OECD, Nimes, France, 25-29 September 2006

CHEN J.C., JUNG P.¹, POUCHON M.A., HOFFELNER W.

"In-situ creep under helium implantation of ferritic ODS steel PM2000"

E-MRS Spring meeting 2006, E-MRS, Nice, France, 29 May - 2 June 2006

¹ FZJ, Jülich, DE

CURTI E., DÄHN R., FARGES F.¹, KUNZ D., VESPA M.

"Ni and Mg redistribution and speciation during alteration of simulated nuclear waste glass: a TEM, μ -XAS and μ -XRF study"

Advanced Light Source Users' Meeting, Lawrence Berkeley National Laboratory, Berkeley, USA, 9-11 October 2006

¹ CNRS UMR, Paris, FR

CURTI E.

"Sorption and precipitation"

2nd FUNMIG Training Course on use of scientific results in site characterisation, Invited Talk, Barcelona, Spain, 23-25 October 2006

DÄHN R., BAEYENS B., BRADBURY M.H.

"Uptake mechanisms of U(VI) by illite as determined by X-ray absorption spectroscopy"

XIII International Conference on X-ray Absorption Fine Structure, Department of Geological and Environmental Sciences, Stanford University, Stanford, USA, 9-14 July 2006

DANG V.H., REER B., PODOFILLINI L., CORAY D.

"A Safety Study for PSI's Proton Therapy Facility Applying Probabilistic Safety Assessment Methods"

Particle Therapy Co-operative Group Conference (PTCOG 44), Zurich and Villigen PSI, Switzerland, 12-16 June 2006

DANG V.H.

"Investigating HRA Methods Using HAMMLAB - Organization of the Benchmarking Study"

Halden Meeting on HRA Method Investigation,, Halden, Norway, 6-7 November 2006

DEGUELDRE C.

"Identification of future colloid/radionuclide/nuclear waste research"

Colloid Workshop, KTH, Stockholm, Sweden, 25-27 September 2006

DEGUELDRE C.

"Zirconia inert matrix for plutonium utilisation and minor actinides disposition in reactors"

CIMTEC 06, Invited Talk, CIMTEC, Acireale, Italy, 4-9 June 2006

DEGUELDRE C., AEBERHARD P.¹

"Modelling of colloid generation/elimination dynamic processes toward a pseudo-equilibrium"

CFM Meeting, IAST, Tokyo, Japan, 12-14 December 2006

¹ EPFL, Lausanne, CH

DEGUELDRE C., KUNZE P.¹, ROSSÉ R.

"Contribution to the study of colloid generation & sedimentation from bentonite FEBEX samples"

CFM Meeting, IAST, Tsukuba, Japan, 11 December 2006

¹ ETH Zittau, Zittau, DE

DEGUELDRE C.

"Status of the Initiative for Inert Matrix Fuel"

Inert Matrix Fuel Workshop 11, INL Argonne, Park City, USA, 10-12 October 2006

DEGUELDRE C.

"IMF challenges after the 11th Inert Matrix Fuel workshop"

Inert Matrix Fuel Seminary, Tokyo Institute of Technology, Tokyo, Japan, 14 December 2006

DEGUELDRE C.

"Zirconia inert matrix for plutonium utilisation and minor actinides disposition in reactors"

Working group meeting on minor actinide transmutation, IAEA, Viena, Austria, 21-23 August 2006

DEGUELDRE C., BART G.

"Nuclear materials: the R&D challenges"

2006 Beijing International Materials Week (2006 BIMW), International Conference on New Energy Materials, Invited Talk, C-MRS, Beijing, China, 27 June 2006

DEGUELDRE C., EWING R.¹, POINSSOT C.², ZHOU L.³

"Nuclear Materials and Materials for Fusion"

E-MRS Spring Meeting 2006, E-MRS, Nice, France, 29 May - 2 June 2006

¹ University Michigan, Michigan, US

² CEA, Gif-sur-Yvette, FR

³ NIN, Xian Schaanxi, CN

DEGUELDRE C.

"Zirconia inert matrix for plutonium utilisation and minor actinides disposition in reactors"

Plutonium Future '06, Invited Talk, Plutonium Future, Monterey, USA, 9-13 July 2006

DEGUELDRE C.

"Single colloid analysis by inductively coupled plasma mass spectroscopy"
INE Seminary, Invited Talk, FZK, Karlsruhe, Germany, 19 January 2006

DEGUELDRE C., KASTORYANO M., DARDENNE K.¹

"VIA-XAFS for the study of zirconia films"

E-MRS Spring Meeting 2006, E-MRS, Nice, France, 29 May - 2 June 2006

¹ FZK, Karlsruhe, DE

DONES R.

"Application of INPRO methodology for assessment of innovative nuclear energy systems"
Technical Cooperation Project INT/4/141, IAEA, Vienna, Austria, 26-30 June 2006

FARGES F.¹, ETCHEVERRY M.², HADDI A.³, TROCELLIER P.⁴, CURTI E., BROWN G.²

"Durability of silicate glasses: an historical approach"

XIII International Conference on X-ray Absorption Fine Structure, Stanford, USA, 9-14 July 2006

¹ CNRS UMR, Paris, FR

² Stanford University, Stanford, US

³ University of Marne la Vallée, St. Denis, FR

⁴ CEA, Gif-sur-Yvette, FR

FOSKOLOS K.

"Swiss Participation in GIF"

Generation IV Workshop, ITU, Invited Talk, Karlsruhe, Germany, 16 October 2006

FOSKOLOS K.

"HTRs zur H₂-Produktion"

Autumn Seminar, Swiss Nuclear Society, Invited Talk, Zurich, Switzerland, 21 September 2006

FROIDEVAL A., SCHUPPLER S.¹, SAMARAS M., VICTORIA M., HOFFELNER W.

"Relationship between the Magnetic and the Structural Properties of Fe-Cr Alloys: XAFS and PEEM Investigations"

Fall MRS 2006, CD-ROM, MRS, Boston, USA, 27 November - 1 December 2006

¹ FZK, Karlsruhe, DE

FU C.¹, SAMARAS M.

"Ab initio study of He in grain boundaries in alpha-iron"

EFDA meeting, EFDA, Lausanne, Switzerland, 7-8 December 2006

¹ CEA, Saclay, FR

GIMMI T., URSINO N.¹

"The concept of dilution and preferential flow and transport in unsaturated media - a critical review of present and past research"

Workshop on Preferential Flow and Transport Processes in Soil, Ascona, Switzerland, 4-9 November 2006

¹ University of Padova, Padova, IT

GIMMI T., WABER N.¹, GAUTSCHI A.², RÜBEL A.³

"Large-scale transport parameters inferred from profiles of natural tracers in pore water of Jurassic argillaceous rocks (Benken, Switzerland)"

4th Swiss Geoscience Meeting, Invited Talk, Berne, Switzerland, 24-25 November 2006

¹ University of Berne, Berne, CH

² NAGRA, Wettingen, CH

³ GRS, Braunschweig, DE

GLAUS M., VAN LOON L.R., YAROSHCHUK A.

"Studies of mechanisms of ion transfer in compacted clay by complementary diffusion and electrochemical techniques"

ELKIN'06, Int. Conference on Electrokinetic Phenomena, Nancy, France, 25-29 June 2006

GONZALEZ F., JURANJI F.¹, GIMMI T., VAN LOON L.R.

"Translational diffusion of water in compacted clay systems"

Confit 2006, 3rd International Workshop on Dynamics in Confinement, Grenoble, France, 23-26 March 2006

¹ Universität Saarbrücken, Saarbrücken, DE

GROLIMUND D., HARFOUCHE M., MEYER B., SCHEIDEGGER A.M., WILLIMANN M.
"The micro-XAS Beamline at the Swiss Light Source (SLS): a New Analytical Facility Dedicated to Micro-Beam Applications"
Annual meeting of the Swiss Chemical Society, Zurich, Switzerland, 13 October 2006

GROLIMUND D., INGOLD G., JOHNSON S., BEAUD P., ABELA R., BRESSLER C.¹, GAWELDA W.¹
"Ultra-fast, time-resolved EXAFS: present capabilities and future prospects"
4th Int. Workshop on Speciation, Techniques, and Facilities for Radioactive Materials at Synchrotron Light Sources, Invited Talk, FZK, Karlsruhe, Germany, 18-20 September 2006
¹ University of Lausanne, Lausanne, CH

GROLIMUND D., HARFOUCHE M., MEYER B., SCHEIDEGGER A.M., WILLIMANN M.
"Status and potential of the micro-XAS beamline"
Int. Workshop on X-ray spectroscopic and microscopic methods, Villigen, Switzerland, 20-21 February 2006

GÜL T., BARRETO L.
"Modelling the Hydrogen Economy with the Energy-System GMM Model"
Responses to Climate Change, NCCR-Climat, Grindelwald, Switzerland, 27 August - 1 September 2006

GÜL T., BARRETO L.
"The Hydrogen Economy: Production Chains, Costs and Analysis with MARKAL"
Before a Transition to Hydrogen Transportation, Joint MIT/PSI Workshop on the AGS Project, PSI, Villigen, Switzerland, 9-10 November 2006

GÜNTHER-LEOPOLD I.
"Characterization of nuclear fuels using destructive and non-destructive analytical techniques"
ZCH Kolloquium (Zentralabteilung für Chemische Analysen), Invited Talk, FZJ, Jülich, Germany, 12 December 2006

GÜNTHER-LEOPOLD I., GUILLONG M., KIVEL N., KOBLER WALDIS J., WERNLI B.
"Characterization of Nuclear Fuels using ICP Mass Spectrometric Techniques"
10th ISMAS Triennial International Symposium on Mass Spectrometry, Invited Talk, ISMAS Indian Society for Mass Spectrometry, Munnar, India, 28 January - 1 February 2006

HARDEGGER P.
"Die Zukunft der Kernenergie in der Schweiz"
Invited Talk, 14th Kantonale Jugendsession, St. Gallen, Switzerland, 1 April 2006

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¹ CNRS UMR, Paris, FR

² Universidad Politecnica de Valencia, Valencia, ES

³ University of Potsdam, Potsdam, DE

⁴ Stanford University, Stanford, US

HASTE T.
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"Nuclear Energy in the UK - The Next Chapter"
Invited Talk, Newcastle University, Newcastle, United Kingdom, 23 February 2006

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"Energy Systems Analysis at PSI"
Seminar for NOK, NOK AG, Baden, Switzerland, 21 April 2006

HIRSCHBERG S.
"Global Warming — A Challenge for Energy Technologies and Policies"
Convention on International Law and Politics, Invited Talk, University of St.Gallen, St.Gallen, Switzerland, 30 November 2006

HIRSCHBERG S.

“External Cost Assessment Methodology, Recent Results and Issues”

Seminar in Energy Economics, Internalisation of External Effects: Theory and Empirics, University of Zurich, Zurich, Switzerland, 10 April 2006

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“Nuclear Energy Risks and Benefits in Perspective”

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“Neue Erneuerbare Energien und neue Nuklearanlagen – Potenziale und Kosten: Erweiterter Beitrag zu den Energieperspektiven 2035/2050 des BFE”

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Fall MRS 2006, MRS, Boston, USA, 27 November - 1 December 2006

HOFFELNER W., SAMARAS M., VICTORIA M.¹

“Modelling Advanced Materials”

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¹ EPFL, Lausanne, CH

HOFFELNER W., SAMARAS M.

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DGMS-2006/ICP-MS Anwendertreffen, DGMS Deutsche Gesellschaft für Massenspektrometrie, Mainz, Germany, 5-8 March 2006

¹ ETHZ, Zurich, CH

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¹ ETH, Zurich, CH

IANNUZZI MAURI M., ROMANO A., SAMARAS M., ZIMMERMANN M.A.

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¹ Hahn-Meitner-Institut, Berlin, DE

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¹ Universität Saarbrücken, Saarbrücken, DE

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“Comparison between Phase-Doppler Anemometry and Shadowgraphy Systems with respect to Solid-Particles Size Distribution Measurements”

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CORS/Optimization Days, Montreal, Canada, 8 May 2006

¹ Lahmeyer International GmbH, Bad Vilbel, DE

KURI G., DEGUELDRE C., BERTSCH J., ROTHE J.¹, DARDENNE K.¹

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¹ FZK, Karlsruhe, DE

LOTHENBACH B.¹, WINNEFELD F.¹, ALDER C.¹, WIELAND E., LUNK P.²

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¹ EMPA, Dübendorf, CH

² Holcim, Zurich, CH

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- MIBUS J.¹, BRENDLER V.², PFINGSTEN W.
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¹ FZK, Karlsruhe, DE
² FZD, Rossendorf, DE
- MIKITYUK K., CODDINGTON P.
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- PELLONI S.
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- POUCHON M.A., KROPF A.J.¹, FROIDEVAL A., DEGUELDRE C., HOFFELNER W.
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¹ ANL, Argonne, US
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- POUCHON M.A., CHEN J.C., FROIDEVAL A., JANOUSCH M., DEGUELDRE C.
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- REER B.
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- RITTER S., SEIFERT H.P., KUMPF K.
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¹ University of Marne la Vallée, St. Denis, FR
² CNRS UMR, Paris, FR
³ University of Paris 6, Paris, FR
⁴ LURE, Paris, FR

SAMARAS M., DERLET P., VAN SWYGENHOVEN H., VICTORIA M.¹
"Atomistic simulations of irradiated magnetic nanocrystalline iron"
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¹ EPFL, Lausanne, CH

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"Ab initio study of He in grain boundaries in alpha-iron"
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TANI F.

“Decomposition Analysis of Reactivity Effect Predictions for Modern LWR Fuel”
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¹ University of Stuttgart, Stuttgart, DE

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² EPFL, Lausanne, CH

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¹ University of Geneva, Geneva, CH

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¹ CSIC-IJA, Barcelona, ES

² ITASCA, Gelsenkirchen, DE

³ University of Berne, Berne, CH

⁴ NAGRA, Wettingen, CH

⁵ Neall Consulting Ltd, Kendal, Cumbria, UK

⁶ Chalmers University of Technology, Gotheburg, SE

⁷ JAEA, Tokai-mura, JP

⁸ Thermo-Calc Software AB, Stockholm, SE

⁹ British Geological Survey, Nottingham NG 125GG, UK

LIST OF PUBLICATIONS

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TEACHING ACTIVITIES (LECTURES)

University Level Teaching

Prof. Dr. U. Baltensperger, Prof. Dr. H. Burtscher, Dr. C. Marcolli
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Dr. P. Jansohn
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 November 10, 2006.

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¹ FHA, Brugg-Windisch

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¹ University of Hong Kong, Dept. of Architecture, Hong Kong, China

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¹ Chonbuk National University, Chonju, Korea

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The catalytic hydrolysis of isocyanic acid (HNCO) in the Urea-SCR process

Ph.D. Thesis, No. 16693, ETH Zürich, June 27, 2006.

M. Santis

Investigation of current density inhomogeneities in polymer electrolyte fuel cells

Ph.D. Thesis, No. 16905, ETH Zürich, October 25, 2006.

W. Scharnhorst

Life cycle assessment of mobile telephone net-works, with focus on the end-of-life phase

Ph.D. Thesis, No. 3443, EPFL 2006.

M. Seemann

Methanation of biosyngas in a fluidized bed reactor. Development of a one step synthesis process, featuring simultaneous methanation, Watergas shift and low temperature tar reforming

Ph.D. Thesis, No. 16754, ETH Zürich, July 19, 2006.

P. Siewert

Flame front characteristics of turbulent lean premixed methane/air flames at high pressure

Ph.D. Thesis No. 16369, ETH Zurich, February 2006.

M. Slaski

Radiation grafted fuel cell membranes with improved oxidative stability

Ph.D. Thesis, No. 16995, ETH Zürich, December 13, 2006.

K. Tikhomirov

Oxidation von Dieselruss in katalytischen Systemen

Ph.D. Thesis, No. 16538, ETH Zürich, April 12, 2006.

H. Turton

Scenario and policy analysis of sustainable energy systems and automobile transportation

Ph.D. Thesis, No. 16886, ETH Zürich, October 25, 2006.

St. van Ekeren

Characterization of an expansion-type cloud condensation nuclei chamber

Ph.D Thesis No. 16944, ETH Zürich, November 2006.

INVITED TALKS

S. Alkan Gürsel

Polymer electrolyte membranes for fuel cells by radiation induced grafting: State of the art at PSI
IRaP 2006, Antalya, Turkey, September 23-28, 2006.

S. Andreani-Aksoyoglu

Differences in SOA in the north and the south of the Alps: A modelling study
The 3rd ACCENT Barnsdale Expert Workshop, Barnsdale, UK, October 31, 2006.

S. Andreani-Aksoyoglu

Fighting against air pollution with modeling tools
University of Waterloo, Canada, August 25, 2006.

S. Andreani-Aksoyoglu

Fight against air pollution. Why is it so difficult?
University of Bilkent, Ankara, Turkey, February 9, 2006.

S. Andreani-Aksoyoglu

Model quality assurance, regional scale
ACCENT Workshop on Model Benchmarking and Quality Assurance, Thessaloniki, Greece, May 30, 2006.

U. Baltensperger

Characterization of atmospheric aerosols with synchrotron radiation
Workshop on x-ray absorption spectroscopy and micro-spectroscopic techniques, Paul Scherrer Institut, February 20-21, 2006.

U. Baltensperger

Klimarelevante Aerosolforschung auf dem Jungfrauojoch
Vortragsreihe für Gymnasiallehrer, Universität Bern, March 1, 2006.

U. Baltensperger

Der Einfluss von Feinstaub auf Gesundheit und Klima
GV Pensioniertenverein PSI, Villigen, December 7, 2006.

U. Baltensperger

Ist der Feinstaub ein altes Thema oder moderne Hysterie?
Parlamentarische Gruppe, Klimaänderung, Bern, December 5, 2006.

U. Baltensperger

Heisse Atome auf kalten Gletschern: Höhenflug des Epiphaniometers
Fest-Kolloquium Heinz Gäggeler, PSI, April 7, 2006.

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Ozon und Feinstaub: Was man beim Sport treiben beachten kann
Ryffel Laufimpuls, Uster, December 5, 2006.

U. Baltensperger

Feinstaub, Quellen und Massnahmen
OcCC, Beratendes Organ für Fragen der Klimaänderung, Bern, March 1, 2006.

U. Baltensperger

Oligomerization in secondary organic aerosol: latest results from smog chamber studies
The routes for organics oxidation in the atmosphere, Alpe d'Huez, France, January 7-11, 2006.

U. Baltensperger

Sekundäre organische Aerosole: Erkenntnisse aus Smogkammer-Experimenten
Feinstaub in der Schweiz, EMPA, Dübendorf, January 20, 2006.

U. Baltensperger

Research on aerosol impact on climate at the high altitude research station Jungfrauojoch, Switzerland
PSI Condensed Matter Colloquium, February 24, 2006.

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Primary and secondary organic aerosols: recent results from smog chamber and field experiments
7th Informal Conference on Atmospheric and Molecular Science, Helsingør, Denmark, June 9-11, 2006.

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Challenges in aerosol research: a perspective from the old Europe and beyond
Aerosol Workshop, Brisbane, Australia, July 5-7, 2006.

U. Baltensperger

Feinstaub in der urbanen Luft: Vorkommen, Eigenschaften und gesundheitliche Relevanz
Fokus Event, Feinstaub in urbaner Luft, ETH Zürich, August 23, 2006.

U. Baltensperger

Primary versus secondary and biogenic versus anthropogenic organic aerosol: grand challenges in atmospheric research
7th International Aerosol Conference, St. Paul, Minnesota, USA, September 10-15, 2006.

U. Baltensperger

Climate relevant aerosol research at the high altitude research station Jungfrauoch, Switzerland
Research at Jungfrauoch - Top of Science, Interlaken, September 11-14, 2006.

U. Baltensperger

What do we need to know about the organic aerosol for air quality and climate
Joint CACGP / IGAC / WMO Symposium, Cape Town, South Africa, September 17-22, 2006.

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Sources and sinks of atmospheric aerosols: impact on regional air quality
aaas Advanced Atmospheric Aerosol Symposium, Milan, Italy, November 12-15, 2006.

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Hygroscopicity and volatility of secondary organic aerosols and related HULIS
Workshop on Humic like substances and their role in the atmosphere, Budapest, Hungary, November 23-24, 2006.

F.N. Büchi

Measuring the current density distribution in PEFC with sub-mm resolution
DaimlerChrysler Forschungszentrum, Ulm, Germany, April 12, 2006.

F.N. Büchi

Fuel cell – supercap hybrid electric drivetrain
F&E Kolloquium, HOPPECKE Batterien GmbH & Co. KG, Brilon, Germany, April 26, 2006.

F.N. Büchi

What is learned beyond the scale of single cells?
210th Joint ECS Meeting, Cancun, Mexico, November 2, 2006.

J. Cozic

Aerosol - cloud interaction: highlights from the Cloud and Aerosol Characterization Experiments (CLACE) conducted at the high alpine research station Jungfrauoch in Switzerland
Alfred-Wegener-Institute, Potsdam, Germany, May 2006.

J. Cozic

The Fate of black carbon in the atmosphere: Its incorporation into cloud droplets and ice crystals
Institute for Atmospheric Science and Climate Science, Zürich, November 2006.

T. Dreier

Linear and non-linear combustion diagnostics
Seminar: Institute for Combustion and Gasdynamic, University Duisburg-Essen, Germany, September 26, 2006.

W. Durisch

Characterization of emitters and GaSb cells for TPV
5th FULLSPECTRUM Plenary Meeting, Freiburg, Germany, June 13, 2006.

W. Durisch

Progress in TPV burners and photoreceivers

6th FULLSPECTRUM Plenary Meeting, Limmassol, Cyprus, November 14-16, 2006.

F. Gassmann

Energie

Primarschule, Meilen, June 9, 2006.

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Einstein's Relativitätstheorie

Zahnärztereverein, Zürich, June 20, 2006.

F. Gassmann

Die wichtigsten Fakten zur anthropogenen Klimaveränderung

Axpo-Besucherführerinnen, PSI-Forum, June 26, 2006.

F. Gassmann

Überblick über die Forschung am PSI

Gymnasium Kirschgarten, Basel, October 25, 2006.

F. Gassmann

Physik, Erkenntnis und Wirklichkeit

Volkshochschule der Region Zurzach, PSI, November 9, 16, 23, 2006.

F. Gassmann

Sieben Hinweise zur Wirklichkeit des Treibhauseffektes

Orientierung für Politiker, Axpo-Besuchspavillon, Böttstein, November 23, 2006.

L. Gubler

PSI Electrochemistry Laboratory: Contributions to efficient energy storage and conversion

EMPA Thun, November 16, 2006.

P. Jansohn

Experimentelle Untersuchungen zur Stabilität von mageren Vormischflammen

Deutsches Institut für Luft- und Raumfahrt (DLR), Stuttgart, January 16, 2006.

P. Jansohn

Programm Kraftwerk 2020

Auftaktveranstaltung, Bundesamt für Energie, Bern, March 29, 2006.

P. Jansohn

Gas turbines for power generation – some recent developments and future trends

Poznan University of Technology, Poland, Celebration of the 150th Anniversary of the Polish Gas Industry, September 25–26, 2006.

G. Knopp

Investigations of perturbations in the ro-vibrational bands of small polyatomic molecules with fs-CARS

Seminar: School of Chemical Physics, International University Bremen, Germany, May 18, 2006.

D. Kramer

Mass transport aspects of PEFCs under two-phase flow conditions

Workshop on Neutron Imaging for Fuel Cells, DaeJeon, Korea, May 12, 2006.

O. Kröcher

Selective catalytic reduction of NO_x with NH₃/Urea over Fe-ZSM5

Lean NO_x Exhaust Reduction Mini Symposium, Corning, NY, USA, November 14, 2006.

S. Kypreos

Stabilising global temperature change below thresholds: a Monte-Carlo analysis with MERGE-ETL

DIW Workshop in Costs of Inaction, Berlin, Germany, March 2006.

S. Kypreos

Integration of country energy system models in a Pan European framework for supporting EU policies
Conference on “Environmental Economics and Investment Assessment”, Mykonos, Greece, February 2006.

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International Energy Workshop (IEW) Cape Town, South Africa, June 2006.

T. Lippert

Laser interaction with materials: from thin film deposition to laser plasma thrusters
Laboratory LP3, University of Marseille, France, March 29, 2006.

T. Lippert

Deposition of thin films
Solid State Chemistry Seminar at EMPA Dübendorf, April 4, 2006.

T. Lippert, L. Urech, C.R. Phipps¹, A. Wokaun

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¹ Photonic Associates, Santa Fe, USA

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Institute of Electronic Structure and Laser, FORTH, Crete, Greece, May 18, 2006.

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E-MRS Symposium Photon-assisted Synthesis and Processing of Functional Materials, Nice, France, June 1, 2006.

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5th International Conference on Photo-Excited Processes and Applications (ICPEPA5), Charlottesville, USA, September 5, 2006.

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Laser-induced backside wet etching: mechanisms and fabrication of micro-optical elements
International Conference on Advanced Laser Technologies (ALT), Brasov, Romania, September 11, 2006.

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Center for Applied Photonics (CAP), University of Konstanz, November 30, 2006.

C. Ludwig

Research needs on pyrolysis and gasification of waste
European Commission, Research Directorate-General, Research in the waste Area – Towards the FP7
Brussels, Belgium, January 31, 2006.

C. Ludwig

Recovering energy and materials from waste and biomass
Environmental Science and Technology Institute, EPF Lausanne, April 3, 2006.

A. Meier

Hochtemperatur-Solarchemie – Sonnenenergie konzentrieren und chemisch speichern
LOG-Kolloquium, PSI, Villigen, August 31, 2006.

A. Metzger

Potential of isoprene to contribute to secondary organic aerosol formation
The 3rd ACCENT Barnsdale Expert Workshop, Barnsdale, UK, October 31, 2006.

P. Novák

Oxygen, hydrogen and CO₂ development in lithium-ion batteries
13th Int. Meeting on Lithium Batteries, Biarritz, France, June 18-23, 2006.

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Interfaces in lithium-ion batteries
Shanghai Jiao Tong University, Shanghai, China, July 18, 2006.

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Relationship between surface chemistry and lithium intercalation properties of graphite
Annual Meeting GFECI-2006, Autrans, France, March 29, 2006.

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Grundlagen und technischer Entwicklungsstand von wiederaufladbaren Hochleistungs-Lithiumionen-Batterien
Workshop Lithiumionen-Batterien in der Automobilindustrie, Hanau, Germany, January 26, 2006.

A.S.H. Prévôt

Aerosole von Holzverbrennung und Verkehr im Misox und in der Leventina (AEROWOOD-Projekt)
Feinstaub in der Schweiz, Dübendorf, January 20, 2006.

A.S.H. Prévôt

New measurement techniques to investigate aerosol composition: Aerodyne aerosol mass spectrometry, accelerator mass spectrometry for ¹⁴C analysis and rotating drum impactor followed by synchrotron-XRF
Seminar of the Transport and Air Quality Unit, Ispra, Italy, February 10, 2006.

A.S.H. Prévôt

The use of ¹⁴C and aerosol mass spectrometry for the characterization of particles
Workshop 'From toxic emissions to health effects', Krakow, Poland, May 15, 2006.

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Messungen und Modellierung im Kanton Uri
Workshop Luft Gebirgstal, Luzern, May 19, 2006.

A.S.H. Prévôt

Air pollution trends around the Alps since 1992
European Geophysical Union, Vienna, Austria, April 6, 2006.

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Spatial gradients of aerosol size distributions near highways studied by mobile on-road measurements
GAeF, Karlsruhe, Germany, June 29, 2006.

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Workshop Wintersmog 2006, Zürich, October 26, 2006.

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Feinstaub, Ozon und andere Luftschadstoffe; Entwicklung, Verursacher und Perspektiven
TCS Sektion Basel, Basel, September 21, 2006.

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Was the changing input of stratospheric ozone responsible for the tropospheric background ozone increase of the northern hemisphere in the 90s ?
American Geophysical Union Fall meeting, San Francisco, USA, December 13, 2006.

P.P. Radi

PHOFEX spectroscopy of H₂CO → H+HCO by DFWM and LIF
Seminar: Prof. Merkt, ETHZ, May 29, 2006.

C.E. Reynolds

Le ratio $\delta^{18}\text{O}$ comme outil pour l'étude de la conductance stomatique des arbres

UQAM - GREFi (Université du Québec à Montréal, groupe de recherche en écologie forestière inter-universitaire), Montréal, Québec, Canada, February 23, 2006.

P.W. Ruch

Time-resolved in situ X-ray diffraction of carbons for supercapacitors

7th SLS Users Meeting, Paul Scherrer Institut, Villigen, September 29, 2006.

M. Saurer

Climate-isotope relationships in tree-rings

Swansea University, Wales, UK, October, 3-5, 2006.

M. Saurer, R. Siegwolf

Human impacts on tree-ring growth reconstructed from stable isotopes

Isotopes as Tracers of Ecological Change, Tomar, Portugal, March, 13-15, 2006.

G.G. Scherer

Recent developments and new trends in radiation grafted fuel cell membranes at Paul Scherrer Institut

Japan Atomic Energy Agency, Quantum Beam Science Directorate, Takasaki, Japan, February 28, 2006.

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NISSAN Research Center, Kanagawa, Japan, March 2, 2006.

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Yokohama National University, Yokohama, Japan, March 3, 2006.

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Combined in situ characterization methods for polymer electrolyte fuel cells

39th Heyrovský Discussion & 7th International Symposium on EIS, Castle Třešť, Czech Republic, June 4-8, 2006.

G.G. Scherer

In situ diagnostic methods for polymer electrolyte fuel cells: Recent progress achieved at Paul Scherer Institut

10th Ulm Electrochemical Talks, Neu Ulm, Germany, June 27-28, 2006.

G.G. Scherer

Aspects of materials research for polymer electrolyte fuel cells

– Keynote Lecture, 57th Annual ISE Meeting Edinburgh, UK, August 27 – September 1, 2006.

– CONAPPICE, Madrid, Spain, September 18-20, 2006.

G.G. Scherer

The potential of in situ diagnostic methods to elucidate the performance of polymer electrolyte fuel cells

Nordic PEMFC 06, Stockholm, Sweden, September 25-27, 2006.

G.G. Scherer

Recent advances in the development of in situ diagnostic methods for polymer electrolyte fuel cells

CEA, Grenoble, France, November 24, 2006.

G.G. Scherer

Materials research for polymer electrolyte fuel cells

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T.J. Schildhauer

Biogas, Biodiesel, Bio-Ethanol: Von der Biomasse zum Treibstoff
Tagung EcoCar, St. Gallen, June 16, 2006.

A. Steinfeld

Solar thermochemical process technology
UOP/Honeywell Invitational Lecture Series, Chicago, USA, March 21, 2006.

A. Steinfeld

Solar thermochemical production of hydrogen
University of Illinois, Chicago, USA, March 20, 2006.

A. Steinfeld

A closer look at the potential of renewable energy sources
VERA Forum, Böttstein, September 18, 2006.

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Renewable Energy
Academia Engelberg, October 9, 2006.

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Thermochemical reactor technology for solar fuels production
LATSIS Symposium, ETH Zurich, October 13, 2006.

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6th Forum Thermo- and Fluid Dynamics, ETH Zurich, November 24, 2006.

Samuel Stucki

Biomasse-Energietechnik
Fernwärme auf neuen Wegen, 5. Tagung, Erneuerbare Energie und Nahwärme, Zürich, January 12, 2006.

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Einspeisung von Methan aus der thermochemischen Biomassevergasung
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- Fachgespräch “Synthetische Kraftstoffe auf Basis Biomassevergasung” des Kompetenznetzwerks “Kraftstoffe der Zukunft” Wuppertal Institut, Wuppertal, Germany, August 31, 2006.
- DVGW-Fachgespräch “Stand und Perspektiven der thermischen Vergasung von Biomasse” E.ON Ruhrgas, Essen, Germany, September 1, 2006.

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Ausblick Forschung Biogas
Tagung Biomethan - Treibstoff aus Biomasse. Umwelt 06, Zürich, September 13, 2006.

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Workshop “Klima- und Biodiversitätskonvention: Konflikte und Synergien” Swiss Biodiversity Forum; Herzberg, Aarau, September 15, 2006.

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Potenzial Bio-Masse in der Schweiz und technische Nutzung

Impulsreferat Retraite der Energiefachstellen der Nordwestschweizer Kantone, Basel, December 6, 2006.

Samuel Stucki

Methanierung von Holzgas

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W.J. Tobler, W. Durisch

Selective emitters for solar and gas-fired TPV systems

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W.J. Tobler, W. Durisch

State-of-the-art of selective emitter developments at PSI

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W.J. Tobler, W. Durisch

Plasma-spray coating of selective emitting rare-earth oxides on intermetallic MoSi₂ substrate

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S. Ulli-Beer

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EMPA, St. Gallen, January 27, 2006.

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B. Verheggen

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J. Vetter

Lithium-ion battery electrolytes - insights and recent progress

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J. Vetter

Application of in situ techniques for investigations in lithium-ion battery materials

210th Electrochem. Soc. Meeting, Cancun, Mexico, October 30 – November 3, 2006.

F. Vogel

Hydrothermal processes for the production of energy, fuels and chemicals – an emerging technology for thermal waste treatment

Seminar on Thermal Waste Treatment, Environmental Science and Technology Institute, EPFL, Lausanne, January 17, 2006.

F. Vogel

Catalytic conversion of biomass to methane in supercritical water

Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, USA, April 27, 2006.

F. Vogel

Technological options for biofuels production

Interdisciplinary seminar on Environment and Agriculture, Graduate Institute of International Studies, University of Geneva, May 17, 2006.

A. Waser

Biomethane - International Outlook

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A. Waser

Bio-SNG: Industrial Demonstration of SNG production technology

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G. Wehrle

Infrastructure and data transfer solution of GAW Aerosol Program at Jungfrauoch

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E. Weingartner

CLACE mission results

Retraite U. Lohmann, Löffingen, Germany, October 16-18, 2006.

E. Weingartner

An overview of the Cloud and Aerosol Characterization Experiments (CLACE) conducted at a high alpine site in the free troposphere

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Erkenntnisse aus dem GAW-Aerosolprogramm am Jungfrauoch

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Überblick über CLACE5

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Activities of PSI at the Jungfrauoch

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A. Wokaun

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European Foundation for the Sustainable Development of the Regions, International Forum 'Electric Power Production', Genève, January 24-25, 2006.

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A. Wokaun

Laufende Projekte des schweizerischen Kompetenzzentrums Energie und Mobilität

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Vision der 2000 Watt-Gesellschaft: Was ist realistisch bis 2050?

Uni Bern Angewandte Physik, December 11, 2006.

PATENT APPLICATIONS

M. Devadas, O. Kröcher, N. Söger¹, M. Pfeifer¹, Y. Demel¹, L. Mussmann¹

Verfahren zur selektiven katalytischen Reduktion von Stickoxiden im Abgas von Dieselmotoren

Patent application, DE102006.016682.5, 2006.

¹ Umicore AG, Automotive Catalysts, Hanau, Germany

T. Gerber

Segmented electrical or optical delay line with interleaved tap for 3D image device readout

European Patent Office, 06005163.8-, March 14, 2006.

Z. Yang, M.G. Roelofs¹, S. Alkan Gürsel, G.G. Scherer

Process to prepare stable trifluorostyrene containing compounds grafted to base polymers using an alcohol/water mixture

WO Patent. 2006.102672A1(2006).

¹ DuPont Central Research and Development, Wilmington, USA

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 31st International Symposium on Combustion, University of Heidelberg, Germany, August 6-11 (2006).

W. Lipinski
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Wasserstoff aus Wasser und Sonnenenergie – Hochtemperatur-Solarchemie
 Electrosuisse Fachliteratur Award 2006
 Electrosuisse Bulletin SEV/VSE **96**, No. 24/25, 11-17, 2005.

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 PSI-Preis für Wissenschaftskommunikation

A. Reiner, G.G. Scherer, A. Wokaun
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Platinum/Carbon co-sputtered fuel cell electrodes
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P. Ruch
Alu-Award 2006.
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A. Steinfeld
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A. Steinfeld
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 für Dissertation "Citizens' Choice and Public Policy. A System Dynamics Model for Recycling Management at the Local Level"

LIST OF PUBLICATIONS

Large Research Facilities

UNIVERSITY LEVEL AND OTHER TEACHING

M. Suter (mit weiteren Dozenten)
Kern- und Teilchenphysik mit Anwendungen
ETH Zürich, WS 2005/2006

M. Suter
Kernphysikpraktikum für Vorgerückte
ETH Zürich, WS 2005/2006

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S. Ivy Ochs
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AMS ^{36}Cl -Measurements at low beam energies

DPG-Tagung, Frankfurt (Deutschland), 13. – 17. März 2006

G. Bonani

Radiokarbondatierung von Milligrammproben mit der Beschleunigermassen-spektrometrie-Methode (AMS)

Institut für Prähistorische und Naturwissenschaftliche Archäologie (IPNA), Universität Basel, (Schweiz), 20.1.2006

M. Christl

Reconstruction of the geomagnetic field strength over the past 300.000 years derived from ^{10}Be data of ODP-drift sediments from the North- and South Atlantic Ocean

Colloquium of DFG Special Priority Program Integrated Ocean Drilling Program, Greifswald (Deutschland), 26. - 29.3.2006

M. Christl

Water mass properties and circulation in the Cape Basin (ODP Site 1089) on Glacial/Interglacial timescale - a multiproxy approach

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M. Christl

^{10}Be in ice cores and marine sediments

Evaluation of Physics Department, Zürich (Switzerland), May 2006

M. Christl

Measurement of ^{10}Be with a compact (<1MV) AMS-facility using BeF^+ ions from BaBeF_4

CRONUS Summer School 2006, Harkany (Hungary), 12. - 17.6.2006

M. Döbeli, M. Mallepell, A.M. Müller, M. Stocker, M. Suter

Will ionization chambers replace silicon detectors for IBA?

CAARI 2006: 19th Intl. Conference on the Application of Accelerators in Research and Industry, Fort Worth, Texas (USA), August 20 - 25, 2006

H. Gäggeler, M. Suter, H.-A. Synal, S. Szidat, L. Wacker

Eine Gasionenquelle für die Niederenergie-AMS

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Cosmogenic nuclide exposure and optically stimulated luminescence dating of glacier extent around the North Patagonian icefield during the Late Pleistocene-Holocene transition

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I. Hajdas

High resolution radiocarbon dating for improved chronologies of paleo records of the last 40 ka

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I. Hajdas

Chronology of Middle Würmian peat deposits from Switzerland—Radiocarbon ages of peat, wood and mammoth bones

Radiocarbon Conference, Oxford (United Kingdom), 5.4.2006

I. Hajdas

The last 50,000 years of climate and human history: ^{14}C time scale as a tool for correlation of terrestrial, marine and ice core records: PAGES ^{14}C Initiative

ESF-IAAMS Workshop "Applications of cosmogenic isotope analysis in earth and environmental sciences", Vienna (Austria), 10.11.2006

I. Hajdas

PAGES ^{14}C Initiative: ^{14}C time scale as a tool for correlation of terrestrial, marine and ice core records

Second Carlsberg Dating Conference, Copenhagen (Denmark) 15. - 17.11.2006

S. Ivy-Ochs

The timing of past glacier expansions in the Alps constrained with cosmogenic nuclides

CRONUS-EU Summer Workshop, Harkany (Hungary), 12.6.2006

S. Ivy-Ochs

Sampling strategies for exposure dating landslides: example the Alps

CRONUS-EU Summer Workshop, Harkany (Hungary), 12.6.2006

S. Ivy-Ochs

Dating past variations in glacier size with cosmogenic nuclides

Quaternary Research Association Annual Discussion Meeting, Glasgow (U.K. Scotland), 5.1.2006

S. Ivy-Ochs

Sample preparation for radionuclides

CRONUS-EU Summer Workshop, Harkany (Hungary), 17.6.2006

T.M. Jenk, S. Szidat, M. Schwikowski, H.W. Gäggeler, H.-A. Synal, L. Wacker

Record of historical anthropogenic and biogenic contributions to carbonaceous aerosols from an alpine ice core

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Multiple cosmogenic nuclides and landscape evolution in the Atavama Desert

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P.W. Kubik

AMS measurements of ^{10}Be and ^{26}Al

CRONUS-EU Workshop, Hannover (Deutschland), 15.3.2006

P.W. Kubik

New developments in AMS technology

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P.W. Kubik

AMS sample requirements for good measurements

CRONUS-EU Workshop, Hannover (Deutschland), 16.3.2006

P.W. Kubik

Accelerator Mass Spectrometry (AMS) measurements of cosmogenic radionuclides
CRONUS-EU Summer School, Harkany (Ungarn), 12.6.2006

M. Mallepell, M. Döbeli

Fast compositional analysis by transformation of ERDA spectra

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A.M. Müller, M. Döbeli, M. Suter, H.-A. Synal, L. Wacker

Accelerator Mass Spectrometry of ^{10}Be at lowest energies

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Beschleunigermassenspektrometrie mit ^{10}Be bei niedrigen Energien

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M. Ruff, L. Wacker, H.W. Gäggeler, M. Suter, H.-A. Synal, S. Szidat, J. Thut

Simplifying radiocarbon measurements with a hybrid ion source at low beam energies

19th International Radiocarbon Conference, Oxford (Great Britain), April 3 - 7, 2006

T. Schulze-König, M. Suter, M. Stocker, H.-A. Synal

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Hochauflösende Gasdetektoren und ihre Anwendung in der AMS

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Smaller and better facilities for AMS – a review of recent developments

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Software und Hardware zur webbasierten Steuerung und Auswertung von Physikexperimenten
GMW06, ETH Zürich (Schweiz), 22.9.2006

M. Suter

Development of compact AMS facilities – Scientific and technical challenges

19th International Radiocarbon Conference, Oxford (Great Britain), April 3 - 7, 2006

M. Suter

Accelerator mass spectrometry - scientific and technical challenges

Seminar at the Adams Institute for Accelerator Science, Oxford (United Kingdom), 5.4.2006

M. Suter

Wie verändern neue Gasdetektoren die Beschleunigermassenspektrometrie

Institutseminar der Universität Wien, (Oesterreich), 23. November 2006

H.-A. Synal, M. Stocker, M. Suter

MICADAS: Ein neuartiges AMS system zum Nachweis von ^{14}C

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DISSERTATION

M. Stocker
AMS bei tiefen Energien
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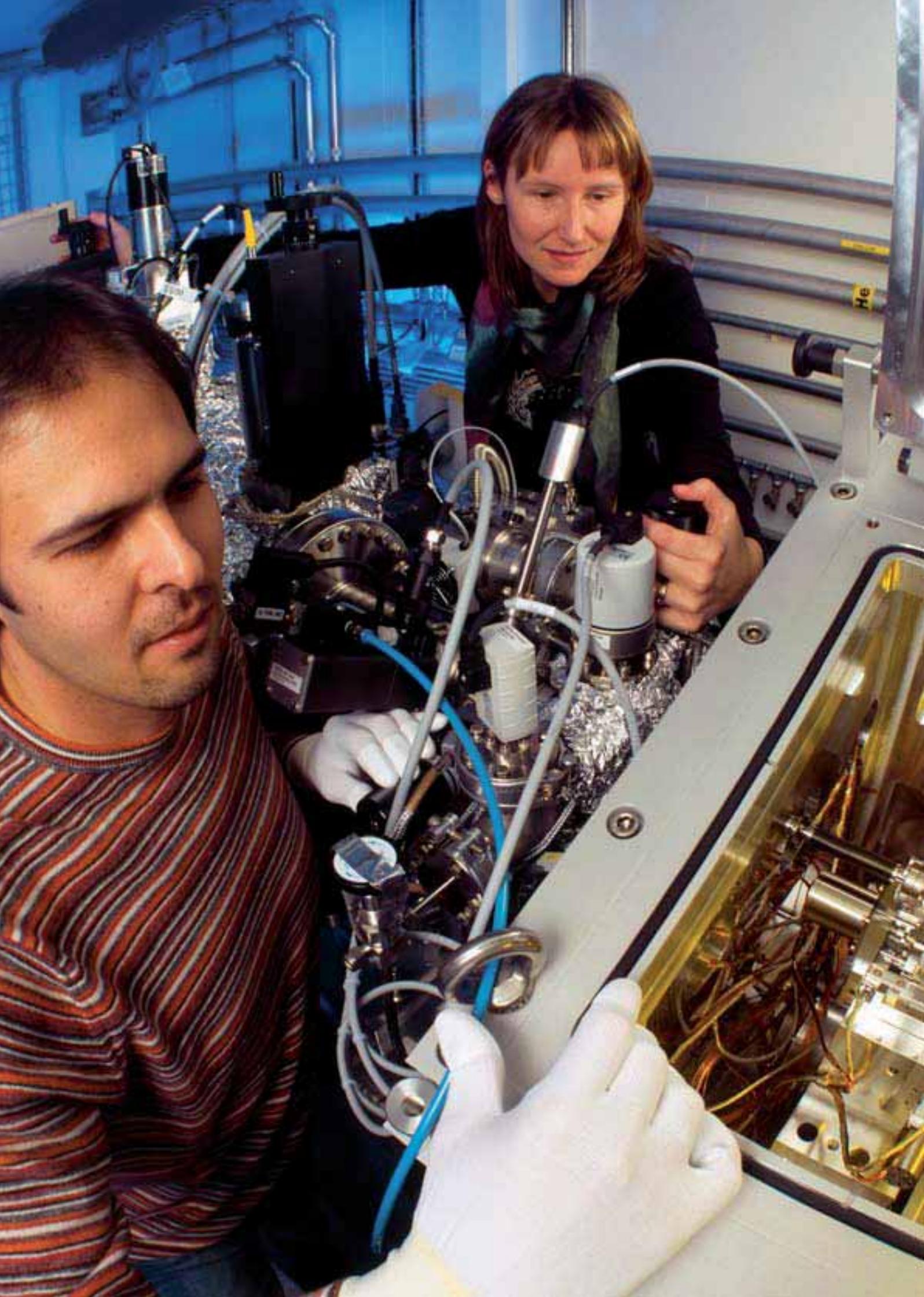
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(Photo: H.R. Bramaz)

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