Abstracts from the Conference

SYNCHROTRON FACILITIES FOR THE DEVELOPMENT OF SCIENCE AND TECHNOLOGY IN CENTRAL AND EASTERN EUROPE

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Lectures

REGIONAL ISSUES SURROUNDING RESEARCH INFRASTRUCTURE

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The regional issue question is closely related to the following questions opened but in no means answered by the contribution:
What is a region?
What is and what can be role of structural funds in promoting regional research infrastructure?
How to promote research at the local level?
How to create atmosphere conductive for the research in new member states competing with classic infrastructure?
How to integrate nationally funded research with EU wide research initiatives?
How to facilitate growth of regionally important research centers into EU large infrastructure?
How to attract investments into regional research infrastructure?

In order to facilitate the answering process the following issues are briefly discussed:

- The role and importance of regions and for regions in the development of a strategic European policy on Research Infrastructures, based on concrete example of policies, institutional arrangements, and/or of existing or planned regional research infrastructures open to international use;
- The expression “regional” applies to nationwide, regional, and local issues
- Identification of gaps in regional research capacities associated with lack of research infrastructure on pan-European level;
- Contribution to the analysis of the socioeconomic impacts of research infrastructures at regional level;
- Potential of regional funding instruments and institutional arrangements for pan-European research infrastructures[1];
- Communication to a wider public about significance and importance of research infrastructures within and for regions.

[1] Over the last decade, the Structural Funds (SF) have contributed to RTD-related investments up to a level equivalent to the Research framework Programme. Within the new financial perspectives (2007 2013) the SF will continue to play an important role, notably by funding activities related to research infrastructures.

CENTRAL EUROPEAN SYNCHROTRON LABORATORY AND OTHER SCIENTIFIC INVESTMENT PROJECTS IN BRNO

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According to the National Strategic Reference Framework the conditions of capacities in research and development including research infrastructure and human capital in the Czech Republic are poor. Real centres of excellence using academic and company capacities for the development of technological disciplines with high growth potential are missing. In addition, research and development capacities are concentrated in Prague.

In order to improve this situation, realization of several large scientific investment projects funded from EU Structural Funds is expected. The establishment of the Central European Synchrotron Laboratory (CESLAB) represents one of them. Another project has been proposed by scientific, research and academic institutions in Brno that decided to coooperate in implemention of Central European Institute of Technology (CEITEC). The CEITEC will consist of four closely cooperating centres of research in the area of life sciences and material sciences and the group of information technologies. The centres will concentrate and integrate capacities in areas of molecular and cell-biology - genomics, proteomics, biochemistry, biophysics, bioinformatics (Mendel Research Centre), biomedical disciplines - molecular oncology, microbiology, stem cells, imagining technology, neuroscience (Biomedical Research Centre), material sciences and advanced technologies - ceramic, polymeric and metal materials and composites, nanotechnology and micro technology in the area of materials and electronics (Centre for Advanced Materials and Technologies) and in veterinary sciences (Centre for Protection of Animals and Humans).

Close collaboration of indivitual centres with CESLAB is expected and synchrotron beamlines will be constructed in order to extend research potential of CEITEC in most advanced fields of research as well as for the development of technologies. For example, advanced imaging using coherent light at synchrotron laboratory will extend possibilities of confocal microscopy in studies of cells, photoemission electron microscopy will extend possibilities of standard electron microscopy, etc. The beamline for nanotechnology will contribute to the CEITEC research in analysis of nanostructures.

Cooperation with other initiatives in the region of a similar type as the ICRC (International Clinical Research Centre Brno) project (medical research in cooperation with Mayo Clinic, USA) is expected.

CONCEPTUAL DESIGN AND BEAMLINES FOR THE NEW CENTRAL EUROPEAN SYNCHROTRON LABORATORY

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The presentation will discuss the conceptual design of the new synchrotron radiation facility to be built in the Czech Republic. It will present proposals for the experimental beamlines with their research fields, applications and the user base.

The new 3 GeV synchrotron to be built in the Czech Republic in Brno will be the 3rd generation source taking the best from the current state of the art of synchrotron physics and technology. The main facility will be based on the latest 3 GeV European synchrotron ALBA, currently under construction. The knowledge transfer, help and direct collaboration on the project planning and later on synchrotron construction has been agreed with the experienced team in ALBA with a support by the respective Czech and Spanish ministries. This considerably boosted preparation of the Conceptual Design Study, which has been in main preparation till October 2007 and it is to be released shortly after a correction phase. From a technical point of view, the storage ring of diameter 270 m will consist of 24 straight sections for insertion devices for up to 33 beamlines.

Beamlines are the heart of results at the synchrotron facility. They provide necessary equipment for the methods applied to different fields of research. They were proposed to support research in biology and medicine, material science, chemistry, microtechnology and nanotechnology, environmental sciences, archeology and other disciplines. The methods of X-ray scattering (high-resolution diffraction, powder diffraction and grazing/small angle scattering), crystallography (single crystals, macromolecules), spectroscopy (absorption, Mössbauer), and imaging (absorption, phase-contrast and coherent, diffraction) will be available at dedicated beamlines. A multipurpose X-ray optics beamline will be available for generic applications, including testing of new components, methods and for metrology. While most of the beamlines will work in the X-ray region, a beamline for VUV chemistry in gas phase and two IR stations for spectroscopy and ellipsometry are proposed as well.

Czech scientists have a long tradition in research with synchrotron radiation. The Czech Republic was the first from the central European countries joining the ESRF, the brightest European synchrotron. Consequently, there is a lot of experience for constructing and running a synchrotron. In the Europe, as everywhere in the world, the demand for beamtime is larger than the available measuring time. A new synchrotron will help to reduce this pressure.

Further, the new source will enhance interest in physics and high technology. It will also allow young researcher easier come-back from their positions in European synchrotrons.

The current trend in the world is to provide fast access for urgent or cutting-edge applications, which is needed mainly for industrial applications. A new synchrotron facility in the favourite location of Brno close to five central European countries will take care of all of these needs.

POLISH NATIONAL SYNCHROTRON CENTRE

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The National Synchrotron Radiation Centre (NCPS) will operate a modern synchrotron light source in Kraków. The project is included in a governmental list of the high-priority initiatives, which will essentially improve and extend the research infrastructure for science and technology on a regional scale. An original design for the accelerator and the storage ring will secure top performance of the facility in its class of medium energy machines. The talk will also outline a scientific case that covers a broad spectrum from fundamental studies in physics and chemistry, applications in material- and nano-science and technology to studies of environmental problems, complex biological systems and medical questions. The advanced research techniques for various disciplines will become available thanks to the specialized beamlines.

THE CYCLOTRON CENTER OF THE SLOVAK REPUBLIC

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The Cyclotron Center of the Slovak Republic (CC SR), as a multidisciplinary project for application of accelerator technologies was established at the beginning of August 1999, within the Slovak Office of Standards, Metrology and Testing (SOSMT), in Bratislava, Slovak Republic. It will have two cyclotrons – a large, heavy and light ion cyclotron DC-72, which was constructed in the Laboratory of Nuclear Reactions in JINR, Dubna, Russian Federation, and a small, commercial light ion cyclotron IBA 18/9.

Modification of material by low and medium energy of ion implantation, ion beam analysis, production of radioisotopes and radiopharmaceuticals and hadron therapy are the main application programs of ion sources of the CC SR. Ion beam produced by the 72 MeV cyclotron DC-72 will be used for clinical treatment of different oncological diseases and for research in the field of radiobiology.

There is a big program to use the CC SR for education on all levels. Activities of the CC SR will be regarded to create in Slovakia a modern scientific-research basis for training of experts from the fields of atomic physics, nuclear physics and techniques, solid state physics, radiochemistry, radiobiology, radiopharmacy and nuclear medicine with the priori aim – to bring new accelerator technologies into practice.

The main purpose of the Cyclotron Center of the Slovak Republic is to catch the present approach and trends in the area of improving of inhabitants life and health quality using the progressive technology, which is introduced by bringing into practice the physical equipment – accelerators, producing beams of high energy particles.

THE EUROPEAN SYNCHROTRON RADIATION FACILITY, 20 YEARS OF EXPERIENCE

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The European Synchrotron Radiation Facility has been created in 1988. Its operation is now financed by 18 European countries. A presentation of the facility will be provided with an introduction to the accelerator infrastructure. The facility has been optimized to provide the most brilliant X-ray beam in the 1 -100 keV photon energy. It includes a 844 m perimeter storage ring circulating a 6 GeV electron beam of low emittance with a full energy injector as well as 43 beamlines range.

The applications of the beamlines cover a large domain including physics, chemistry, biology, nanotechnogy, medical applications, environmental science, cultural heritage. The scientific production has steadily increased and now results in more than 1500 refereed publications every year. The presentation will also focus on the Financial, Technical and Academic "Fall-out" from the ESRF of which the Grenoble and the local region have largely benefited.

SCIENCE WITH SYNCHROTRON RADIATION AT FORSCHUNGSZENTRUM KARLSRUHE

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The 2.5 GeV synchrotron light source ANKA of Forschungszentrum Karlsruhe enters its fifth year of operation and ranks as a national German user facility.

Embedded in the rich scientific infrastructure of Forschungszentrum Karlsruhe, ANKA mainly focuses on the use of synchrotron radiation in the science areas of

- Condensed Matter
- Nano- and Microtechnologies
- Actinide Research and Environmental Research
- Synchrotron Technology

In these fields the ANKA user service will increasingly be complemented by versatile techniques of fabrication, processing and characterization provided by institutes of Forschungszentrum Karlsruhe.

ANKA´s scientific impact is enhanced by links with excellent universities, institutes of the Max Planck Society and the Fraunhofer Society, Joint Research Centres of the European Commission such as the Institute for Transuranium Elements (ITU), and European institutions such as the European Synchrotron Radiation Facility ESRF in Grenoble, as well as through collaboration with industrial partners.

Apart from approx. 3500 hours of beamtime for public use, about 300 hours of accelerator operation at lower electron energy were delivered for special applications including the so-called low-alpha mode, allowing the generation of extremely compressed bunches down to a length of 150 μm at 1.3 GeV. The short bunches are the basis for the delivery of coherent synchrotron edge radiation (CSER) in the so called THz gap. In this mode the superconducting undulators also provide short, 500 femtoseconds X-ray pulses with a high repetition rate of 500 MHz. At a total current up to 30 mA these are the shortest X-ray pulses presently available at a storage ring source.

ANKA - undulator program

Financed by an EU Joint Research Activity and by additional funding of the Helmholtz Association, and strengthened by contractual collaboration with industry, the superconducting insertion devices program is entering the phase of prototype development for third generation low emittance storage rings. Detailed investigation at ANKA is presently focusing on heating mechanisms of the cooled vacuum chamber inside the undulator, on the shimming technology and on the construction of quality-control set-ups, e.g. for magnetic field measurements.

ANKA will equip all its long straight sections with superconducting insertion devices, one of them with electrically switchable period length and one with electrically switchable polarization.

Upgrade ANKA beamlines

After years of high scientific success of the infrared beamline IR1, construction of the second infrared beamline IR2 will allow to further augment the number of experiments in this energy range at ANKA. IR2 will be dedicated to IR-microspectroscopy and near field microscopy, whereas IR1 will focus on ellipsometry, high pressure and low temperature experiments. At both IR beamlines coherent THz radiation is available for experiments.

Two insertion device based beamlines are in the design and ordering phases, respectively. Their measuring stations funded by the state of Baden-Württemberg will profit from superconducting undulators: NANO for high resolution and interface sensitive scattering methods and IMAGE for X-ray imaging methods based on absorption, phase and diffraction contrast. We thank the international community of users and experts for having supported the formulation of the scientific case and the beamline design within two international workshops.

New Collaborative Research Projects at ANKA

In 2007 the universities of Karlsruhe, Bochum, Erlangen and Freiburg started projects of instrumental and methodological development at ANKA in the fields of near field infrared microscopy, in-situ X-ray scattering, X-ray pixel array detectors and superconducting undulators within a collaborative research programme of the Federal Ministry of Education and Research.

At European level, two new consortia of research institutes, universities and industry have taken up their work at ANKA: ANKA is co-ordinator of the ScinTax collaboration, which develops X-ray array detectors with novel ceramic thin film based scintillators for high resolution imaging. The SIDAM project develops X-ray methods for calibration of in-line X-ray inspection methods optimized for microelectronic fabrication.

SYNCHROTRON LIGHT SOURCE FACILITIES: IMPORTANCE AND SPECIFICITY OF COMMUNICATION

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This talk focuses on the aspects of communication in the area of synchrotron based science and technology. Three subjects are dealt with: 1. /External communication./ This includes all information targeted at the public that is not familiar with synchrotron light science at different background levels, from the non-scientist (general) public (local, non-local public, politicians, students, teachers, journalists from the various media) to the non-specialised scientists (physicists, engineers, chemists, biologists, geologists, palaeantologists, etc.). Messages (=> aims) are: i) synchrotron light sources are extremely useful tools to study problems important to our society and to innovate => attract/ensure funding: a SLS is an excellent investment in the present and the future; ii) synchrotron light sources address a huge range of research and development activities and offer outstanding experimental opportunities => attract users, also from industry; iii) synchrotron light sources are superb places for scientists to work => attract excellent scientific collaborators; iv) synchrotron light sources cover a great variety of science and technology and lend themselves to science education practices => attract the younger citizens to enroll in scientific careers; All these /outreach and education /activities aim to increase the level of scientific understanding and promote science in general. They represent the return in /knowledge/ of the investment in /capital/. 2. /Internal communication: the user community/. Present and future users are regularly informed about the present state of both the individual facility and all facilities world wide, about experimental opportunities, scientific programmes, staff, important visits, workshops and conferences, collaborative projects and agreements, seminars, experimental results formulated as press releases, etc. This includes also /inter-facility communication/ issues such as common developments, projects, exchange programmes, etc. 3. /Internal communication: the in-house staff/. In a larger scale scientific institution it is important to create social coherence and thus to enhance motivation by informing staff members about the mission of the facility, in particular on what is behind the words used by scientists, typed by secretaries and appearing in publications. In addition to the information about social events, salary increases and safety rules, a good in-house culture supported by /intra-facility communication /must necessarily include a good general knowledge on the importance and usefulness of the science produced by the institute. An overview of the different communication tools such as press releases, visits, audio-visual documents such as videos, seminars, brochures, internet activities, e.g. the portal /lightsources.org/ and various events is given too.

GIVEN THE SCIENTIFIC QUALITY, WHAT ELSE IS NEEDED TO MAKE A REGIONAL RESEARCH FACILITY A SUCCESS STORY?

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When political decisions are taken to build an Infrastructure, the general tendency (i.e. by Regional and National Financial Authorities) is to think to financially self-sustaining infrastructures, i.e. those (like an Highway or a Manifacturing Plant, etc.) which, after construction, generate an income capable to cover the operation and the maintenance costs, and possibly also are able either to refund the investors or to compensate the decrease of value (amortization or upgrades). This self sustainability is *never* reached by a Research Infrastructure, and this normally comes as a surprise to the funders, generating a very difficult political atmosphere within few months after the beginning of the operation phase. This is in part due to the confusion between Research, Development and Innovation, which affects several levels of Policy Making and Industry.

Research is, by definition, unable to self sustain, and the experience shows that a Research Infrastructure will be able to cover only a fraction of its operation costs of less than 10% (most often less than 5%) differently from Development or Innovation activities which can generate incomes comparable to the costs. Unless a Research Infrastructure is funded by research money (contributions without return by a Government, Academy or other not for profit Institution) a fully comprehensive analysis of the "indirect" socioeconomic returns is necessary to detail what is the advantage to invest in it.

The definition of the socioeconomic returns requires that, both the Infrastructure itself *and the surrounding region,* are considered in a comprehensive project where the conditions for the generation of values, different and complementary to those of Research, are accounted for. We will present some aspects of this approach.

THE ACCELERATOR COMPLEX FOR THE ALBA PROJECT

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The accelerator complex of ALBA exist as in other third generation light sources of a pre accelerator, booster synchrotron, storage ring, the transfer lines, the corresponding transfer lines, the front ends, and the insertion devices. The pre accelerator is a 135 MeV turn key linac optimized for a small energy spread and minimum electron losses. For the booster synchrotron we took over the concept from the Swiss Light Source and having it together with the storage ring in the same tunnel. The lattice for the booster synchrotron is however different (TME structure) in order to get smaller damping times and emittance, which could be reduced by a factor 2. It is a full energy injector capable for top up injection. The storage ring with an energy of 3 GeV has a circumference of roughly 270 m, the lattice design was determined by the condition 1.) to have small cross section of the beam and 2.) to have a lot of straight sections. The lattice of the storage ring is a DBA structure with combined function bending magnets (gradient = 5.8 T/m) in order to get a compact magnetic structure. The emittance of the storage is 4.3 nmrad with overall 24 straight sections: 4 long (8 m long), 12 medium (4.3 m long), and 8 short (2.3 m long). Overall 38 % of the circumference is devoted to straight sections. The medium straights have so called "mini beta section" to reduce the size of the stored beam. The radio frequency system with normal conducting cavities is designed to store a beam of 400 mA.

ADVANCED DETECTORS FOR NSLS-II

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NSLS-II will be the brightest storage ring light source in the world when it begins operation in 2014.

The parameters of this machine will be briefly discussed. Then, current and proposed research into advanced detector systems will be described. These systems will allow more efficient use of the photons generated and will allow new science to be performed.

SOLEIL, A NEW MEDIUM ENERGY THIRD GENERATION FACILITY FOR THE EUROPEAN SCIENTIFIC AND INDUSTRIAL COMMUNITIES

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SOLEIL is now in operation with 11 Phase I beam-lines starting to accommodate their first users and already open to the European scientific community. The other 16 Phase II beam-lines are at various stages of their construction and installation; all of them will be in operation by mid 2010. After a year of commissioning of the storage ring, most of its characteristics are better than specified and the electron beam stability is already in the micron range. I will present a brief status of the characteristics and performances of the storage ring and of the Phase I beam-lines, as well as a few examples of innovations developed at SOLEIL that might be of interest for the 3 GeV Czech project.

SOLEIL is a medium energy facility (2.75 GeV) which intends to be complementary of the high energy ones available in Europe, the ESRF and soon PETRA III. It has been designed to be the brightest in the soft and tender X-ray ranges, though it is still an excellent light source up to 20 keV on the high photon energy side and down to 5 eV on the low energy one. The choice to cover such a broad energy range results from the scientific needs expressed by the community of the users through more than forty workshops. They required that about half of the beam-lines be devoted to the investigation of the electronic properties of matter using mainly IR, VUV and soft X-rays, the other half being hard

X-ray beamlines mostly dedicated to structural studies. This balanced program is one of the specificities of SOLEIL in comparison with other new third generation synchrotron facilities.

Another of its characteristics is the large number of beam-lines (11) dedicated to imaging and micro- and nanospectroscopies using all the energy ranges. It is partly due to the strong demand of these techniques for societal and industrial applications, like environment, medicine, pharmaceutics, food science and industry, nano-technologies. The use of SOLEIL for cultural heritage will be particularly important with the installation on its site of a new institute dedicated to the field, IPANEMA, open to the European users by 2009-2010. The implementation of another new institute focussing on structural and cellular biology, with a strong interface with pharmaceutics, has also been decided by the Paris Sud University to boost the life sciences at SOLEIL.

Since similar needs may be expressed by the scientific and industrial communities in Central and Eastern Europe, I will briefly review the main characteristics of the SOLEIL scientific program as well as those of the foreseen applications. Some information will also be given on the construction and operation costs, the manpower, the strong collaboration with the local authorities, as well as some personal views on management issues derived from a 6 years experiencewith the design, construction and installation of SOLEIL.

NANOSCIENCE@MEGAFACILITIES.EUV REPORT FROM THE GENNESYS STUDY

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Little happens in industrialised countries without the use of high-tech materials which are the building blocks of all modern technologies ranging from information, communication, health, energy to environment and transport. Through our microscopic insight into the atomistic structure of condensed matter, the development of novel materials has progressed at a breathtaking pace during the last decades.

Breakthroughs in the future development of advanced materials and novel technologies are facing key barriers in the destruction-free insitu analysis of nanomaterials and nanomaterial systems under industrially and environmentally relevant conditions. These barriers pose critical challenges onto modern European Synchrotron radiation facilities which have developed an impressive analytical potential and which are ready to offer and adjust their analytical technology to the advancement of nanoscience and nanotechnology.

In this lecture, I review the conclusions and recommendations of the GENNESYS foresight study [1] on the future development of nanoscience and nanotechnology exploiting modern European Synchrotron radiation and neutron facilities.

1. GENNESYS Grand European Initiative on Nanoscience and Nanotechnology using Neutron and Synchrotron Radiation Sources (appears 2007).

SYNCHROTRON RADIATION IN PROTEIN CRYSTALLOGRAPHY. OPPORTUNITIES FOR PROTEIN CRYSTALLOGRAPHY AT CESLAB

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The scientific use of synchrotron radiation and applications of results of the protein structure analysis in economy, medicine and health care were the cause that 17 sources of synchrotron radiation were build in the western part of the European Union, providing thus more than 30 diffraction beamlines for advanced measurements in this part of Europe. Opposite to the rapidly growing number of synchrotrons in the western part of EU, the eastern part of Europe (Czech Republic, Poland, Slovakia, Slovenia, Hungary, Austria, Bulgaria, Rumania, Latvia, Estonia, Lithuania) have no experimental equipment of this type by now.

Medical and biological sciences in the Czech Republic are on high level and also structure biology results are promising - almost 10 % of all complexes of HIV protease deposited in the PDB were published by Czech groups; the structure of protein with the lowest R factor was refined by Ondráček et al, 2007 [1]; structure determination of large macromolecular complexes (Skálová et al, 2006) [2], etc.

However, the critical lack of experimental time at sources of synchrotron of radiation has been serious obstacle in development of modern science. Two planned diffraction beamlines in Brno are optimized for structure determination of biomacromolecules. One beamline is optimized for quick, reliable and accurate structure determination of large molecular complexes. The second beamline has tunable wavelength and is specialized to MAD, SAD structure determination, reliable location of ions in structure, and other specialized tasks.

Macromolecular Structure Beamline - 1 (MSB-1) operates with an undulator optimized for the use at the fixed wavelength ~ 1 Å . The X-ray optics offers diameter of primary beam 10 to 200   m with optimum for ~ 50   m. The precise microdiffractometer with more circles will allow 100 % completeness of the collected experimental data. Automated sample changer, cryocooling, in-line microscope and high speed CCD detector (read-out time in parts of second) with large detection area optionally allows a continuous data collection without use of the shutter.

Macromolecular Structure Beamline - 2 (MSB-2) operates with an undulator tunable in a range of wavelengths 0.6 – 2.0 Å. The precise microdiffractometer with the automated sample changer, cryocooling, in-line microscope, and fluorescence detectors. The X-ray optics have optimum characteristics for diameter ~ 50   m. High speed

CCD detector with large detection area optionally allows a continuous data collection.

The users of the macromolecular beamlines need also well equipped laboratories: physical and chemical laboratory (microscopes, lasers), biochemical laboratory (crystallizer, incubators, storage boxes, freezer, microscopes), cold room (microscope, storage boxes) and computing room (terabyte data storage and high-speed transmission of data).

In spite of the fact that the design of the macromolecular beamlines in Brno is economic, it will provide more services than it is usual at the standing synchrotron facilities. It will also ensure new advanced technologies necessary for structure determination of large molecular complexes, and for identification of ligands or ions in biopolymers.

1. J. Ondráček *et al*, unpublished results.
2. T. Skálová, J. Dohnálek, E. Vondráčková, H. Petroková, V. Spiwok, P. Lipovová, H. Strnad, B. Králová, J. Hašek, *J. Mol. Biol.* **353** (2005) 282-294.

CARBOHYDRATE-BINDING PROTEINS: A WAY TO UNDERSTAND RECOGNITION PHENOMENA IN LIVING SYSTEMS

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Biomolecular interactions play a crucial role in living systems where they are used not only for recognition but they are involved in information transfer and communication in living system in general. Carbohydrate-mediated recognition is important in many physiological processes including fertilization, pathogen-cell adhesion and recognition, signaling, inflammatory response and others.

Protein-carbohydrate interactions are usually characterised by a low affinity for monovalent ligands that is balanced by multivalency resulting in high avidity for substrates with several potential ligands available, such as complex glycans or cell surfaces. Therefore, understanding of these processes requires a detailed structural information about all the partners involved.

Contribution will be focused on some examples of sugar-binding proteins from pathogenic organisms showing how important is a possibility to see the protein/ligand complexes on the atomic level. Insight into binding sites and further correlation with thermodynamics of interactions gives a high potency for further pharmaceutical and biotechnology application.

SYNCHROTRON RADIATION FOR BIOMEDICAL IMAGING AND RADIATION THERAPY

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Medical application of synchrotron radiation (SR) is a fast-growing field of research. Since the advent of the angiography studies at SSRL first and then at NSLS in the U.S. in the 1990s, preclinical and clinical research protocols have been developed at Hasylab (Germany), Photon Factory (Japan), ELETTRA (Italia) and at the ESRF (France). Despite the fact that there are only a few dedicated beamlines in the world (two new ones are under construction at the Australian and Canadian synchrotrons), medical research is carried out in almost all synchrotron facilities. Biomedical research at SR facilities has many purposes. Basic research is carried out for diagnostic and/or curing purposes using the ideal experimental conditions offered by a SR source (monochromatic and collimated beam, etc.). A second objective is to develop innovative techniques that can be directly applied in clinical trials at SR sources, and that in the future can be used at new generation table-top X-ray sources presently under development worldwide. In this frame, the ID17 ESRF Biomedical Beamline was built in the 1990s with the aim of developing two specific programs: the Transvenous Coronary Angiography and the Microbeam Radiation Therapy. Thanks to the increase of the users' community, the beamline activities are now also extended to and focused on functional (e.g. lung and brain) and anatomical (e.g. breast and cartilage pathology) imaging, and radiotherapy (including basic radiobiology). All imaging programs are presently in the preclinical development, while radiation therapy programs, namely the Microbeam Radiation Therapy (using spatially fractionated white X-ray beams) and the Stereotactic Synchrotron Radiation Therapy are approaching the clinical phase. A review of the research opportunities offered by SR will be here presented and discussed.

SYNCHROTRON RADIATION X-RAY FLUORESCENCE ANALYSIS: MEDICAL, ENVIRONMENTAL AND INDUSTRIAL APPLICATIONS

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Energy dispersive X-ray fluorescence analysis using synchrotron radiation as excitation source offers several advantages in elemental analysis in comparison to standard X-ray tube excitation: higher photon flux, wide spectral range for efficient excitation and linear polarization in the orbital plane for background reduction. Using Total Reflection geometry (SR-TXRF) ultra trace analysis can be extended to samples with only small sample amounts available (e.g. aerosol samples) or wafer surface contamination control. Using grazing incidence XRF (GIXRF) also determination of depth profiles and implantation dose determination is possible nondestructively (ultra shallow junctions). Synchrotron radiation focused to a microbeam of about 10 m allows also spatial resolved 2 D imaging of various samples (e.g. trace element distribution in human bones will be shown). Using the confocal setup with a second focusing element in front of the detector extends the imaging to 3 D as the volume where the information comes from can be precisely determined and scanned. Samples of human joint bones will be presented. Exchanging the standard multilayer monochromator with laregg band width by a crystal monochromator with high energy resolution absorption spectroscopy measurements (XANES or EXAFS) can be performed in fluorescence mode and combine the before mentioned features of trace element analysis with information about chemical speciation. Examples of speciation of Iron in aerosol samples, Arsenic in xylem sap of cucumber plants and Pb in human joint bones will be presented.

CHEMISTRY IN THE GAS PHASE: FROM CHEMISTRY OF INTERSTELLAR SPACE TO ORGANOMETALLIC CATALYSIS

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Investigation of the properties and the reactivities of ions in the gas phase has proved as an important tool for the basic chemical knowledge. Mass spectrometry – the leading method for the ion gas-phase studies – is able to provide valuable information about structures, stabilities, and energetics of ions. Combination of tandem mass spectrometry with photoionization using synchrotron radiation brings a unique possibility to control the internal energy of ions formed and represents therefore a truly powerful technique. The VUV photons provided by the synchrotron have well-defined energy and are smoothly tunable, which allows not only for accurate determinations of ionization and fragmentation thresholds, but also sophisticated studies of internal energy effects and state-specific reactions. As a result, the synergy of photoionization methods using synchrotron radiation and modern mass spectrometry provides accurate and reliable benchmarks for organic reaction mechanisms, transition-metal catalysis, atmospheric as well as interstellar chemistry, and - of course - also analytical chemistry.

Relevant examples from groups having high interest in the use of a Czech Synchrotron are: 1) The determination of barrier for the keto-enol tautomerism of acetamide (D. Schröder, IOCB, Prague). 2). Reactivity studies of molecular dications (Z. Herman, JHI, Prague / J. Roithová, CU, Prague). 3) Thresholds for photoionization and fragmentation of metallocenes (B. Sztaray, ELU, Budapest). 4) Recent improvements of models of planetary atmospheres of Mars, Venus, Titan, and Earth (O. Dutuit, France, EUROPLANET). Finally, it should be stressed that the studies using synchrotron radiation provide valuable benchmarks for thermochemical studies and theoretical calculations, which both is highly appreciated not only in fundamental research, but also in applications for industry.

SYNCHROTRON RADIATION BASED STUDIES FOR ORGANIC ELECTRONIC APPLICATIONS

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During the last decade huge efforts was performed to realise electronic devices based on organic semiconductors. A variety of electronic and optoelectronic prototypical devices was realised and currently some of them are nowadays used in practical applications. E.g. organic electroluminescence is used in flat panel displays or thin film transistors are used as active elements in large area projection screens. However, the knowledge about the underlying physical effects is still poor and a large scientific community is working in this field to get detailed understanding of the physical and chemical properties in organic semiconductor devices.

The talk will present the outstanding electronic, optical and structural properties of organic semiconductors and the difference to inorganic semiconductors will be discussed. Some open questions will be addressed and current progress by using synchrotron based experiments will be shown. The examples will be taken from the nowadays most prominent organic semiconductors like pentacene, sexithophene and sexiphenyl.

ULTRAFAST IMAGING OF MAGNETIC SWITCHING PROCESSES UTILISING THE TIME STRUCTURE OF SR

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Fast processes on the sub-nanosecond time scale and transient states in nanoscale electronic systems are attracting high interest in basic and applied research. The excellent time structure of Synchrotron radiation is an ideal tool to study such processes. Time resolution in the range of a few picoseconds can be achieved in stroboscopic full-field photoemission electron microscopy (PEEM) with high lateral resolution [1]. Remagnetisation processes and transient domain states or magnetic high-frequency eigenmodes in confined magnetic structures [2-4] are of interest due to challenging applications, e.g. in spintronics. Implementation of a time-of-flight technique into the microscope column provides a novel approach to spectroscopic imaging and opens way for aberration correction [1].

In this contribution the state-of-the-art of time resolved PEEM for the observation of transient magnetic domain states and high-frequency excitations is discussed. Stroboscopic imaging of precessional magnetic switching utilises X-ray circular magnetic dichroism (XMCD) as contrast (magnetic field pump / X-ray probe). At the storage ring BESSY (Berlin), a time resolution of about 15 ps has been obtained [2]. Fast magnetic field pulses are generated by passing fast current pulses through a coplanar waveguide thus yielding field amplitudes of several Oerstedt above the stripline. This set-up allowed the observation of spin waves, both standing eigenmodes as well as propagating modes, in confined thin-film elements of permalloy ($Ni_{80}Fe_{20}$). Magnetic thin-film structures are fabricated via lithography on top of the waveguide. At grazing incidence we are most sensitive to the in-plane magnetization component along the photon beam. The phase front of a spin wave propagates at 8100 m/s, being much faster than typical domain wall velocities in permalloy.

We have also studied ultrafast magnetodynamics in micropatterned spin-valve structures fabricated in an industrial environment (NAOMI Sensitec GmbH, Mainz) [5]. The magnetic multilayer stack was excited with field pulses of 250 ps width. The dynamic response of the “free layer” (the layer that switches) falls into two distinctly different contributions: On the one hand, it exhibits localised spin wave modes that strongly depend on the shape of the micro pattern. On the other hand, the integrated responseof the free layer roughly follows a single-macrospin model with a damping constant of = 0.025 (independent of the shape) and resembles the response of a critically damped forced oscillator. Such kind of information is of utmost importance for tailoring the optimum switching behavior of, e.g. magnetic memory elements (M-RAM).

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OPPORTUNITIES FOR THE DEVELOPMENT OF STATE OF THE ART IMAGING TECHNIQUES AT CESL

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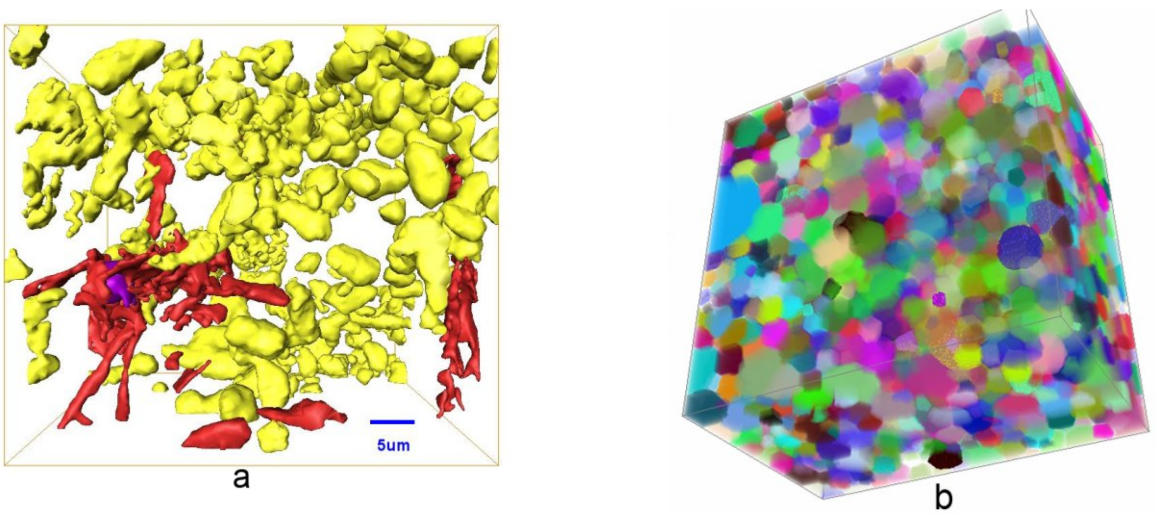
High brilliance, tunability and large lateral coherence of the X-ray beam emerging from 3rd generation synchrotron sources opens a venue for scientists to study the structure and dynamics of a wide range of samples. Particular studies require high spatial or temporal resolution, or both. These two aspects of synchrotron imaging will be addressed here.

As an example we show on Figure 1a that nanoscale zoom-tomography with hard X-rays can reveal the structure of composite materials and moreover reconstruct the shape of micrometer size features with spatial resolution better than 300 nm in the hard X-ray range. When performing such experiments, the limitations of nanoscale tomographic techniques in terms of the focusing optics, thermal and mechanical stability have been recognized. These are crucial parameters to consider when designing experimental stations such as the planned imaging beamlines at CESL.

Driven by the desire to study the dynamics of rapidly evolving systems, substantial effort has been put into the reduction of scanning time in tomography mode. Through optimization of the acquisition system the efficient use of the high brilliance of the synchrotron beam allowed to reduce scanning time by a factor of roughly 10 over the past 3-4 years. Figure 1b depicts a subvolume of a liquid foam at a well defined time. The evolution of liquid foams represents an example of experiment which could not have been performed without this progress towards faster image acquisition.

All the experiments presented here have been performed at the ID19 beamline at ESRF. These examples can represent the motivation to establish cutting-edge imaging techniques at the newly planned CESL.



a)

Figure 1 (a) 3D phase map of an Al-Si alloy highlighting the Iron-rich inclusion (dark/red) between the Si particles (light/yellow). The image is acquired in divergent beam setup, the resulting effective voxel size is 50 nm. (b) Labeled individual bubbles of a rapidly evolving liquid foam. The whole volume of 2048 1024 pixels scanned in fast tomography mode with scanning time of 25 s, on the figure we show a region of 700 700 300 at pixel size 7.5 microns.

SYNCHROTRON FOR X-RAY OPTICS & X-RAY OPTICS FOR SYNCHROTRON

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Imaging X-ray optics is a key element of numerous scientific instruments such as large astronomical space X-ray telescopes, X-ray microscopes, etc. The recent trend of achieving high intensity and superior imaging quality in future projects with X-ray optics requires reliable and easily available test instruments with focus on tests using X-ray beams. Here the synchrotron X-ray beam lines play an important and still increasing role. At the same time, some special X-ray optics can have wide and important application in synchrotron facilities, especially as fine focusing elements allowing achieving small spot sizes and high intensity. Related projects and efforts in the collaboration of several Czech institutions in these directions will be presented and discussed.

RECENT ACTIVITIES AND STATUS OF THE SPECTROSCOPY BEAMLINES AT SPRING-8

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Although SPring-8 is a high energy accelerator whose energy is 8GeV, some spectroscopy beamlines covering from infrared to hard-X-ray energy range exist. The public beamlines are opened to world wide users. Two soft X-ray beamlines (200~2000eV) are used for solid state spectroscopy and gas phase spectroscopy, respectively. Angle-resolved photoemission provides us bulk-sensitive information of band structures and the Fermi surface structures in detail. Photoemission electron microscope is mainly used for magnetic domain imaging together with the micro-XAFS measurements.

Recently, time-resolved measurements combining with the fs laser pulse becomes possible, which give us dynamical information of matters. Magnetic circular dichroism in soft-X-ray absorption spectra is widely used not only by university researchers but also by industrial companies. We have started soft-X-ray emission spectroscopy, too. The gas phase spectroscopy community using this beamline is very active. Coincidence measurements with photoelectrons and photo-ions, and time of flight measurements for dissociative fragment show us a detailed mechanism of the photoexcitation process of atoms and molecules. Some hard-X-ray beamlines (5~10keV) at SPring-8 are applied for photoemission measurements. Because the photoelectrons excited by such high energy light have large kinetic energy, information obtained by this method is really bulk sensitive. In some case we do not need to prepare clean sample surfaces.

The infrared spectroscopy beamline is mainly used for micro-spectroscopy. Recently we have started the R&D of near-field microscopy. The setup of beamlines, their characteristics, and representative activities are introduced.

SYNCHROTRON-RADIATION ACTIVITIES IN NANOSTRUCTURES AND NANO-MATERIALS IN CZECH REPUBLIC AND NEIGHBOURING COUNTRIES: OPPORTUNITIES FOR NANOTECHNOLOGIES AT CESLAB

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For the investigation of structure of very small objects like quantum dots, crystalline nanoclusters, and other types of nanostructures, synchrotron radiation is a essential tool making possible to reveal positions of atoms in these types of objects, as well as their chemical composition, elastic strains and other structural parameters. The uniqueness of the synchrotron radiation consists not only in this extremely high brilliance compared to conventional laboratory X-ray sources, but also in its energy tunability, excellent coherence properties, and its ideal polarization. For the study of nanostructures, a variety of synchrotron-based experimental methods is used, ranging from "conventional" high-resolution X-ray diffraction and reciprocal-space mapping to X-ray spectroscopy methods like EXAFS, XANES and DAFS, X-ray standing-wave method, X-ray fluorescence and X-ray-induced photoelectron spectroscopy. Recently new types of nanostructures have been developed and new experimental methods emerged, such as coherent X-ray scattering including phase retrieval, and micro- and nano-beam scattering.

Parallel to the development of nanostructures and characterization methods, a substantial progress has been achieved in synchrotron instrumentation – not only in large facilities like free-electron lasers, but also in commercially available small intense x-ray sources (“table-top synchrotrons”).

In the talk, I will review synchrotron-based studies of nanostructures in Czech Republic and neighboring countries, presenting several examples of experimental results. Based on an overview of these activities at several synchrotron sources available so far and on the expected development in the synchrotron instrumentation in future, I will critically discuss the necessity of building a new synchrotron in Central Europe in general and in Czech Republic in particular.

COUPLING, ANISOTROPY AND DOMAIN STRUCTURE IN METALLIC MULTILAYERS

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Antiferromagnetically (AF) coupled metallic multilayers (ML) have received much attention and appreciation in recent years, including the 2007 Nobel Prize in physics, due to their relevance in fundamental science and magnetic recording technology alike. Both their plane-perpendicular and lateral magnetic structure can be efficiently studied by two closely related nuclear scattering techniques, see synchrotron Mössbauer reflectometry (SMR) and polarised neutron reflectometry (PNR). Here we present SMR studies of the magnetic-field-history-dependent formation and transformation of magnetic domains in a strongly AF-coupled epitaxial ML.

The orientation of the magnetisation of the ferromagnetic layers can be measured to a high accuracy by the specular intensity of the AF reflections. This fact has been used to demonstrate the bulk-spin-flop transition in a strongly AF-coupled Fe/Cr ML. The value and distribution of the critical field of this transition reveal details of the layer-layer coupling, in-plane magnetic anisotropy and domain-wall motion, all playing decisive role in the performance of magnetoresistive devices.

The off-specular (diffuse) reflectivity probes the in-plane component qx of the scattering vector and, consequently, reveals the in-plane correlation length of the scattering amplitude. Starting with a strongly AF-coupled ML in magnetic saturation and then gradually decreasing the field, two kinds of AF patch domains differing only in the sense of rotation of the magnetisation in their odd and even layers are spontaneously formed. On further decreasing the field and, thereby, increasing the domain-wall angle, the size of the domains is expected to spontaneously increase in order to decrease the domain-wall energy per unit area of the ML. We observed this domain ripening with SMR and evidenced a relatively sudden growth of the domain size from 370 nm to 800 nm. The domain ripening was found to be an irreversible process (up to saturation) and was also followed by an apparent change in the shape of the diffuse scattering peak.

A dramatic increase of the domain size from 800 nm to at least 5 m, i.e., a coarsening of the AF domains was observed in the same multilayer when it passed the BSF transition provided that the external magnetic field was previously decreased from magnetic saturation to zero. This shows the key role of the in-plane magnetocrystalline anisotropy in the domain-coarsening process. In contrast to ripening, a domain-wall-energy-driven and coercivity-limited process, the explosion-like coarsening is driven by the Zeeman and the anisotropy energies and is not associated with any long-range domain-wall movement. Akin to ripening, also coarsening was found to be irreversible as long as the applied field did not reach the saturation region.

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SOFT X-RAYS: THE ELETTRA EXPERIENCE

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Elettra is the first medium energy third generation synchrotron source built in Europe. It is operational since 1995. It was developed as a source complementary to the ESRF and its scientific case was primarily in the VUV-soft X-rays range. A number of beamlines in this energy range have been developed at Elettra during the years aiming at the characterization of a number of materials, including surfaces, interfaces, thin films, nanostructures using photoelectron spectroscopy based method (time, space and/or kresolved), imaging methods and photabsorbtion. During the talk examples of such applications will be given. After over 10 years of operation the user community is still growing and new applications arebeing developed extending the methods to other disciplines, such as lifesciences.

APPLICATION OF SYNCHROTRON RADIATION IN RESEARCH OF STRUCTURAL MATERIALS: OPPORTUNITIES FOR MATERIAL SCIENCES AT CESL

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The structural materials form the framework of the human society starting from the building stones up to nanoelements in electronic devices. Experimental techniques based on application of synchrotron have been becoming importance in the advanced research of structural material namely from the point of view of micro and nanostructure research of dynamic processes.

Starting from the heavy industrial application, in-situ observations of the dynamic evolution of microstructures during the welding of commercial alloys are now possible because of a novel synchrotron radiation-based X-ray diffraction technique. Synchrotron radiation, in the form of an intense highly collimated X-ray beam, can be focused into a sub-millimeter sized beam to probe atomic structures in time scales of milliseconds rather than the hours required by conventional sources [1].

New information on early stages of surface oxidation (corrosion) was obtained using photoelectron spectroscopy where the light source is synchrotron radiation (UPS). As an example, detailed investigation of the surface layer on electrotechnical steel sheets will be presented [2]. Precise analysis of the Si-2p photoelectron peak profile discovered presence of new iron-silicon intermetallics in the upper layer.

Research on high density recording media (terabytes hard discs) is focused on Fe-Pt materials in form of nanoobjects with requested structure and magnetic properties. To understand principles of their magnetic behavior X-ray magnetic circular dichroism and EXAFS based on application of synchrotron radiation were applied [3]. This study explained the correlation between size and the element-specific magnetic moments.

Carbon nanotubes attract attention for their extraordinary physical properties which can bring important progress in nanoelectronics. Actual research is focused namely on their preparation in large scale with well defined sizes and properties. Investigation of the $Si/SiO_2/Fe$ substrate using UPS showed new information on behavior of the iron thin layer during temperature increase in the process of carbon nanotubes growth [4].

The short overview of applications of synchrotron radiation in research of various structural materials show that this modern experimental tool can bring new data which help in development of novel structural materials with improved quality.

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SYNCHROTRON RADIATION USERS COMMUNITY IN POLAND - ORGANIZATION, SCIENTIFIC INTEREST, SCHOOLS AND CONFERENCES

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The First Meeting of the Polish Synchrotron Radiation Users took place on 11-12 February 1991 in Krakow. It gathered 34 researchers from several scientific institutions in Poland that actively exploited the synchrotron radiation in their research. The idea of creating the Polish Synchrotron Radiation Society (PSRS) was born there. On 5th of May 1991 the PSRS was officially registered with Prof. Andrzej Kisiel as the first president. Today PSRS has 121 active members and 20 foreign members. The main goal of PSRS activity is to support a development of the research with the use of the synchrotron radiation (SR) and a popularization of this kind of research in Poland. The means used to achieve these goals are first of all the organization of National Meetings of the Polish Synchrotron Radiation Users (PSRU) in order to integrate the SR users community and to have the overview of their scientific activity. Next the organization of the International Schools and Symposia on Use of Synchrotron Radiation in Natural Science (ISSRNS) in order to teach the young scientists in the advanced use of SR based methods. During the 16 years of the PSRS activity eight ISSRNS and seven PSRU were organized, and six other conferences devoted to the use of SR were co-organized by PSRS in Poland. Moreover two workshops devoted to the EXAFS technique took place in IoP in Warsaw each gathering more then 60 young scientists from scientific institutions in Poland. Several other specialized workshops are being planed in the nearest future. Starting from 2002 the Bulletin of PSRS is published. Six volumes of the Bulletin were published till now.

A recently built database containing papers with application of SR published by scientists having Polish affiliation exceeds one thousand one hundred. One can notice a fast increase of the number of papers and Ph.D. theses with studies involving the SR. During the period of 1998-2005 only at the Hasylab, Hamburg, 164 Polish projects were performed. This long lasting activity of Polish scientific community in the application of SR finally found a support from the Polish government. Starting from July 2004 Poland is officially a member of ESRF, and from July 2006 is an associated member with the share of 1%. Polish government is supporting the access of Poland to the European Free Electron Laser in Hamburg. The project of creating the Polish National Synchrotron Radiation Center is under preparation and has got a green light from the Polish government.

In the lecture the activity of the Polish scientific SR community will be presented and the exceptional examples of the research performed by Polish scientists with the use of SR will be shown.

SYNCHROTRON - VUV AND XUVRADIATION

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Synchrotron radiation (SR) has become a very important tool in many branches of science. Current SR sources generate radiation continuously tunable across the wide region of the electromagnetic spectrum. The SR is also highly polarized and collimated in a very narrow forward cone. With these features, SR provides which is currently applied in surface physics, materials science, chemical, biological and medicine research. Dedicated SR sources optimized to generate VUV and XUV radiation are mostly applied in spectroscopy and microscopy. As main experimental tools in these field methods based on photoemission, absorption of radiation or imaging with emitted electrons or X-rays offers new possibilities and improve substantially tasks commonly used in conventional laboratories. We will give a brief survey of methods mostly used in this spectral region to study electronic structure, chemical state and composition, local structure and microscopy with the chemical resolution.

UTILIZATION OF SYNCHROTRON RADIATION AT THE INSTITUTE OF PHYSICS SAS AND SYNCHROTRON COMMUNITY IN SLOVAKIA

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Synchrotron radiation (SR) has become an indispensable tool for several research lines conducted at the Institute of Physics of the Slovak Academy of Sciences. Quantitative high-resolution structure analysis of short-range ordering and size distribution determination of nanocrystalline grains in amorphous metastable matrix using SR is of vital importance for development of new nanomaterials with unique properties at the Department of Metal Physics. Development of new spintronic nanostructures based on giant or tunneling magnetoresistance (GMR, TMR) effect with current-induced magnetization switching (CIMS) at the Department of Multilayers and Nanostructures [1] has brought qualitatively new demands for characterization of interfaces in multilayers and hybrid structures as well as self-assembling effects of magnetic nanoparticles. SR offers unique possibilities for probing self-assembling effects and interfaces in terms of morphology and interface magnetism.

The lecture will exemplify each of these three applications of SR presenting some recently obtained results. Firstly, effect of the deposition technique on the interface morphology in terms of power spectral density will be documented by -GISAXS measurements (HASYLAB, BW4 beamline). Secondly, self-assembling effects in the evaporating drop of a nanoparticle solution will be traced by static as well as time-resolved -GISAXS combined with SAXS to answer the questions where the nanoparticle ordering takes place and what the final nanoparticle array looks like [2] (HASYLAB, BW4 beamline). Thirdly, a proof of the induced magnetic moment in gold in Au/Co multilayers deposited by two different techniques based on XMCD and XMRS measurements will be shown. Having 5d band filled completely in the atomic form, gold can acquire magnetic moment only via electron hybridization at the interfaces which produces spin-polarized 5d holes. Consequently, the induced magnetic moment is extremely small and difficult to detect in this particular case (ESRF, ID12 beamline).

The lecture will also introduce some present and potential users of SR in Slovakia with their respective fields of interest and will give a personal assessment of the author of Slovak possibilities to participate at construction of CESL beamlines.

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SYNCHROTRON RADIATION OPTICS AND INSTRUMENTATION IN THE REGION

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Laboratories and companies in the Czech Republic (and partially in neighboring countries), developing methods and instrumentation applicable for synchrotron radiation are briefly described.

STRUCTURE AS A KEY TO FUNCTION: PROTEIN ENGINEERING AND MOLECULAR MODELING OF LECTIN-SACCHARIDE INTERACTIONS

Adam, J.[1], Pokorná, M.[1], Sabin, Ch.[2], Kříž, Z.[1], Imberty, A[2], Koča, J.[1], Wimmerová, M.[1,3]

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Solving protein structures and analysing the relationships between structure and function of a protein is a keystone of biomolecular chemistry. The understanding of the connections between them is crucial e.g. for the process of protein engineering – designing proteins with precisely defined and desired properties. Having a protein structure solved enables also the application of powerful computational chemistry and molecular modelling methods in order to model and predict the behavior of the biomacromolecules in silico, potentially saving the experimental time by helping to choosing promising directions in advance. Synchrotron radiation offers one of the most precise and effective ways of solving crystal structures of the proteins. The study is focused on lectins, proteins capable of binding saccharide structures with both high affinity and specificity, deciphering the sugar code information.

The lectin PA-IIL from *Pseudomonas aeruginosa* plays an important role in the bacteria's virulence. It is able to bind fucose with micromolar affinity, thanks to unusual binding mode mediated by a pair of calcium ions. Similar structures have been found in other bacteria, with different binding preferences despite only slight sequence changes. Mutations of the PA-IIL were designed according to these differences, performed and investigated both in vitro, and in silico [1]. Thanks to the ESRF facility, it was possible to measure and solve the crystal structures of the PA-IIL and its mutants [2,3], correlate the structural data to the thermodynamics, and compare them to the results of the computational study. Overall, the study helped to reveal the crucial role of the amino-acid composition of the binding site for binding preferences, and the possibility of in silico prediction of these interactions. The structural knowledge paired with computational chemistry can therefore be of great help in protein engineering and drug design.

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INFRARED SPECTROSCOPY (ELLIPSOMETRY) WITH SYNCHROTRON RADIATION

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We report on ellipsometric measurements in far-infrared range using a synchrotron radiation. We discuss advantages of a synchrotron radiation with respect to standard sources. Results on high-temperature superconductors are shown. Other infrared spectroscopy techniques (microscopy, high pressure, high magnetic field) that take large advantage of synchrotron radiation are briefly discussed.

ORDERED 2D SYSTEMS OF ORGANIC MOLECULES AND NANOPARTICLES IN LANGMUIR MONOLAYERS AND LANGMUIR-BLODGETT FILMS

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Organic materials are of great interest for electronic applications, as they have many advantages over their inorganic counterparts. They may often be solution-processed, allowing the fabrication of devices such as circuits, displays, and biosensors. The most attractive prospect is the incorporation of functionality by design. Since the electronic and optical properties of organic thin film material are intimately connected to the packing motifs of the molecules in the films, it is of paramount importance to achieve control of the assembly process that take the molecules from a disordered state in solution into the ordered condensed state on a substrate. An ideal tool for studying the self-assembly process of molecules or nano-sized objects in two-dimensions is offered by the Langmuir-Blodgett (LB) technique, which allows formation of a monolayer on the water surface and a subsequent transfer onto the solid substrate preserving the molecular order achieved in the monolayer.

The air/water interface provides some unique opportunities to study self-assembly processes. First, the "substrate" (water) is extremely well defined, because it is flat and homogeneous, second, the effective dimensionality of the assembly process is reduced from 3 to 2 dimensions and the molecules are free to move only in the lateral direction, and third, recent developments of synchrotron sources, providing very intense X-rays, have allowed diffraction experiments to be performed directly on monomolecular films floating at the air/water interface [1]. This type of experiment allows the in-plane structure of the monolayer film to be elucidated. Once the films have been transferred to solid substrates, local probe methods, such as AFM, SEM, TEM may be used for studying the in-plane structure of the film surface. In combination, these two types of methods bring detailed information on topography of 2D system, which is important for determining its electronic or optical properties.

This presentation documents some particular examples of results of X-rays diffraction and X-ray reflectivity measurements from LB layers formed of lipid molecules, which are models of biological membranes, of nanoparticles, and of organic molecules (diacetylene, parylene), which belong to organic semiconductor and insulator classes. In all cases, this approach proved itself as a powerful tool for acquiring direct in-plane structural evidence. The results are confronted with microscopic images.

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GALLIUM STRUCTURE ON SILICON SURFACES STUDIED BY SYNCHROTRON RADIATION PHOTOELECTRON SPECTROSCOPY

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The influence of temperature, adsorbed water and hydrogen on the structure and behaviour of gallium atoms on silicon surfaces studied at Materials Science Beamline of Elettra Synchrotron Light Laboratory in Trieste is presented and summarized [1–3]. The gallium structure was monitored by low-energy electron diffraction (LEED) and synchrotron radiation photoelectron spectroscopy (SR-PES). A detailed analysis of photoelectron spectra was carried out and different Ga 3d and Si 2p peak components were recognized and related to gallium or silicon atoms in different positions and/or bonding arrangement.

In the case of gallium deposition on Si(111)-(7×7) surface [1] it was found that the deposition at room (or lower) temperature leads to a non-ordered growth up to a critical coverage (around 1.5 ML), beyond which gallium forms small droplets on the silicon surface. At higher temperatures either only the island bases were formed (over 490 °C) or these bases were covered with extra gallium atoms in an additional layer (300 °C) with metallic properties. In addition to the previously reported structures, a new (3 3 × 3 3) R30° reconstruction was observed after high temperature deposition followed by annealing to 530 °C. This structure was stable in a narrow temperature range and forms an intermediate step between the (3 3) R30° reconstruction and the island structure.

The results on Ga deposition on a clean Si(100)-(2×1) at a higher temperature (490 °C) [2] are consistent with a Ga ad-dimer model showing the equivalent bond arrangement of all Ga atoms for coverages up to 0.5 ML. The gallium deposition onto a surface with adsorbed water at room temperature [2] led to a disordered growth – gallium atoms bind to silicon dimers already binding fragments of adsorbed water. A subsequent annealing of these layers leads to a surface structure similar to the Ga-(2×2), however, it is less ordered, probably due to the presence of silicon oxides formed from water fragments. Further, it was found that gallium deposition on Si(100)-(2×1)-H surface at elevated temperature [3] leads to hydrogen desorption and formation of the same gallium surface phases as on bare Si(100)-(2×1).

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ACTO-MYOSIN MOLECULAR MOTOR AS A ‘LIVING CRYSTAL’: AN INVESTIGATION OF STRUCTURAL STATES BY TIME-RESOLVED SYNCHROTRON RADIATION DIFFRACTION

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Contractile cells can exert their main function, cell motility, owing to the presence in them of filamentous proteins, mainly myosin and actin, and the highly-ordered fashion of the proteins’ assembly. As such, they can be considered ‘living crystals’ and investigated in much the same way as other crystalline specimens, e.g., by X-ray diffraction.

The acto-myosin molecular motor operates in a quick cycle consisting of four main states (‘strokes’). The structure associated with some of them was investigated in crystallised isolated myosin motor domains/subunits (subfragments 1 or S1) [1]. While these experiments are precise from a classical crystallography perspective, they say nothing about force generation associated with such states, as encountered in the living tissue. The present investigation aims to probe this ‘uncertainty relation’, by studying the molecular motor directly in situ in a tissue preparation.

The preparations (ca 5 mm long and 0.5 mm in diameter) were dissected either from frog sartorius or rabbit psoas muscle, and permeabilised with a mild detergent (1% Trixon X-100), to make their cytosol accessible for experimental manipulation [2]. The individual states of the molecular motor were arrested (‘chemically frozen’) by various ATP analogues (ALF_{4-}, AMP.PNP, vanadate or pyrophosphate). Upon irradiation with an X-ray beam (ca 4 0.5 mm in crossection, wavelength 0.15 nm), the 3rd meridional X-ray diffraction signal was recorded (M3, 14.5 nm^{-1}), as it samples the S1 subunit’s orientation [3]. To simulate the working cycle of the motor domain (S1), dynamic, time-resolved X-ray diffraction experiments were performed in some states, by applying mechanical oscillations to the tissue preparation (0.1 or 1.0 kHz).

In rigor state, the final step of the molecular motor’s working cycle, the oscillations were also applied on top of a step stretch which was meant to force the motor domain out of its standard mean orientation. As a result of this additional experimental perturbation, the M3 time-course pattern became, in some preparations, comparable to that observed in intact (non-permeabilised) preparations in a different functional state, namely in the activated state. The present data thus helped to remove one of several variables still present in the complex molecular motor equation set.

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STRUCTURAL BASIS OF SIX BLADED -PROPELLER LECTINS AAL AND RSL

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The lifestyle of bacterium and fungi like saprophytes, symbiotes or pathogens require the specific recognition of organics matter or host issues for adhesion and subsequent invasion. A common strategy adopted by bacteria and fungi involves binding to host glycoconjugates using sugar-binding proteins, lectins [1].

This contribution describes two fucose binding lectins: AAL (312 amino acids) - the fungal lectin from *Aleuria aurentia* and RSL (90 amino acids) – the bacterial lectin from *Ralstonia solanacearu*m. The crystal structure of AAL - the first structure of fungal lectin – was found to be a six bladed ß-propeller with a small antiparallel two-stranded ß-sheet that plays a role in dimerization. Five fucose residues are located in binding pockets between the adjacent propeller blades [2].

The bacterial lectin RSL displays strong sequence similarity to one-third of the sequence of the AAL lectin. The RSL monomer is composed of two four-stranded ß-sheets and assembles as a trimer, forming six-bladed ß-propeller fold very similar to that of AAL [3]. Although the ß-propeller fold has been observed now in many protein families, RSL is the only example in all protein space to date in which the torus is generated by oligomerization and not by peptide repeats of the same continuous protein chain.

Each RSL monomer has two binding sites, one intramonomer and one at the interface with the neighbouring monomer, for a total of six sites per trimer. The ligand-binding sites of AAL and RSL are very similar, and are characterized by numerous hydrogen bonds to the side chains of polar amino acids and by strong hydrophobic interaction between aromatics residues. The similarity at the sequence, structural and binding site levels between fungal lectin and bacterial one could be due to the gene exchange allowed by close contact of the two organisms in soil.

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STANDING-WAVE EFFECTS IN GRAZING-INCIDENCE X-RAY DIFFRACTION FROM POLYCRYSTALLINE MULTILAYERS

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The intensity of X-ray diffraction from a polycrystalline multilayer in a grazing-incidence scattering geometry is modulated by a standing wave created by the interference of the radiation transmitted through the multilayer stack with the wave field specularly reflected from the superlattice interfaces. Similarly, the radiation being diffracted from the polycrystalline structure is reflected specularly from the interfaces and a standing-wave interference pattern results as well. The standing-wave effects in diffraction from polycrystals have been analyzed theoretically in [1].

This effect is demonstrated by a series of diffraction measurements on Ni_3N/C periodic multilayers; the experimental data have been modelled using the distorted-wave Born approximation and a very good correspondence with the experiments was achieved. We have found that the Ni_3N layers are not polycrystalline in the whole volume and the shape of the grains depends on the layer thickness. We have also determined the dependence of the grain sizes on the depth of the Ni_3N layer in the multilayer stack.

The measurements of the reflectivity curves and powder diffraction in classical symmetric geometry were performed using a standard laboratory setup; GID measurements were carried out at the ID01 beamline at ESRF, Grenoble.

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RESONANT INELASTIC X-RAY SCATTERING OF TRANSITION METAL COMPOUNDS

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We measured resonant inelastic X-ray scattering spectra at the K-edges of several transition metal compounds (Ti, V, Mn, Fe, and Cu) with a high-resolution in-vacuo Rowland-circle spectrometer [1] that has been installed at the DORIS III storage ring in HASYLAB. The spectrometer utilizes either spherically or cylindrically bent silicon crystals of several orientations to analyze the fluorescence signal outgoing from the sample. The measurements are preferably performed in a dispersive set-up with a sample located inside a Rowland circle and with position sensitive detector on the circumference of the focusing circle. The spectrometer works at fixed Bragg angle, the energy transfers are obtained by varying the incident photon energy. The energy resolution of the spectrometer is about 1 eV.

Resonant inelastic X-ray scattering (RIXS) is a two photon process with an intermediate state at the low unoccupied valence electron states a provides similar kind of information as X-ray absorption spectroscopy. The advantage of RIXS is that by tuning the excitation energy through the absorption edge of the observed element the high resolution fluorescence spectra are obtained. The fluorescence spectra excited close to threshold show significant differences, and allow to separate transitions, which cannot be separated with conventional X-ray absorption spectroscopy. For site-selective spectroscopy, K fluorescence measurements are generally better suited than K fluorescence, because due to the non-negligible overlap of 3p-electrons with the valence electrons, the energy and line-shape of the K fluorescence lines depend on the oxidation state and on the ligand. On the other hand, in order to separate and identify the transitions into unoccupied states in the near-edge region, the measurements of K fluorescence lines are preferable.

Here we present 1s3p RIXS spectra (Kß fluorescence lines) of titanium dioxide (TiO_2), both rutile and anatase, and the 1s2p RIXS spectra (K fluorescence lines) of vanadium pentoxide (V_2O_5). The RIXS measurements for TiO_2 were performed for excitation energies from 4965 eV to 4980 eV (step 0.5 eV) and reveal the well separated structure consisting of three pre-edge peaks. The pre-peaks are broadly assigned as Ti 1s-4p dipole and 1s-3d quadrupole transitions that are influenced by strong O 2p – Ti 3d hybridization. Surprisingly the position of the first pre-peak for both compounds is shifted to lower energies, although the incident energy has been tuned above the excitation threshold yet. Similarly, we measured 1s2p RIXS of V2O5 for excitation energies from 5460 eV to 5480 eV. We observed a sharp resonance in the fluorescence spectra at the energy of 5467 eV. The resonance can be assigned to the doublet structure, which can be seen in the conventional XAS only as a weak feature in the derivative absorption spectrum. The structure was for the first time described by Wong *et al*. [2] and was interpreted as effect from crystal field splitting.

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TEMPERATURE STABILITY OF GE RICH SIGE STRUCTURES

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Si and Ge alloys are becoming more and more important in semiconductor industry due to their application in electronic and optoelectronic devices and due to progress in Si/SiGe strain engineering [1]. Indeed the production, processing and operation of device create a large thermal load, which induces thermal instability of the produced structure. The heat dissipation in the circuits and devices operation at high temperatures requires the knowledge of the diffusion processes.

A series of investigations of diffusion in SiGe have been done, unfortunately the interdiffusion process in SiGe alloys is non-linear and strongly depends on Ge content [2,3]. Detailed parameters describing precisely SiGe intermixing were measured in literature for low Ge content in SiGe structures, but the data for Ge rich SiGe are missing with sufficient precision.

The aim of our investigation is to extend the knowledge about $Si_{1-x}Ge_x$ interdiffusion process for the range of Ge content x from 50 % to 100% and to determine new values of diffusion coefficients of SiGe for various Ge concentrations. In order to obtain both the activation energy EA and diffusion prefactor D0, series of isothermal annealing at various temperatures is necessary to perform. We have annealed simple $Si_{1-x}Ge_x$ multilayers (x = 70% and 90%) grown by molecular beam epitaxy on relaxed SiGe pseudosubstrates with constant composition of Ge. The multilayers consist nominally of 10 periods of SiGe quantum wells and barriers, covered by an additional SiGe cap layer in order to preserve the strain symmetrization.

We have investigated the diffusion properties of SiGe multiple quantum well structures using *in-situ* diffraction techniques at asymmetric coplanar geometry performed at

ESRF at beamline BM20. The structural parameters as lattice constants, strain and Ge content profile were determined from simulations of 224 diffraction pattern obtained at elevated temperature. The critical temperature, where the interdiffusion starts to be observable, is in the range from 600 °C to 700 °C. Thus we have collected series of reciprocal space maps at several temperatures mostly around 650 °C. The temporal evolution of diffraction pattern will allows us to determine the diffusion coefficients for various temperatures, from which we can extract the activation energy and strain status of the material for given concentration of germanium in SiGe. We have observed that the rate of interdiffusion increases with increasing Ge content as expected from previously published results.

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KINETICS OF CRYSTALLIZATION IN Fe-BASED NANOCRYSTALLINE ALLOYS STUDIED BY DIFFRACTION OF SYNCHROTRON RADIATION

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Disordered nature of structural arrangement in amorphous and nanocrystalline alloys gives rise to advantageous (from a practical application point of view) magnetic properties [1]. Especially nanocrystalline alloys attract a lot of scientific interest because, contrary to their amorphous counterparts, their magnetic parameters do not substantially deteriorate at elevated temperatures during the process of their practical exploitation. To benefit from their unique magnetic properties, the mechanism of crystallization should be known. Here, we present the study of kinetics of crystallization in a NANOPERM-type alloy by the help of diffraction of synchrotron radiation during continuous heat treatment. Till now, only few studies were devoted to in situ study of crystallization of metallic glasses [2]. Our investigation makes use of very fast acquisition of diffraction patterns which is especially suitable for dynamic studies.

Alloys of the composition $Fe_{91-x}Mo_8Cu_1B_x$ with x = 12, 15, 17, 20 prepared by rapid quenching on a rotating wheel were analyzed in the as-cast state. Monochromatic synchrotron radiation of 7 keV (= 1.78 nm) provided at the KMC-2 beamline at BESSY Berlin was used for in situ examinations of structural transformations during continuous heat treatment. As-quenched samples were placed inside a vacuum furnace and exposed to temperature increase with a ramp of 10 K/min up to 800 C. Diffraction patterns from a 2 region covering the main (110) bcc Fe reflection were recorded every 10 seconds using a 2D detector.

After suitable processing, the data were analysed and plotted as 2D images with the time of heat treatment being the second parameter. As an example, the resulting image obtained from the wheel side of the x = 12 ribbon. The onset of the first (T_{x1}) and the second crystallization (T_{x2}) step is indicated. The overlaid line shows the evolution of the temperature measured at the sample's surface with the time (right-hand scale) of acquisition of the 2D diffraction pattern.

Diffraction lines positioned at about 52.5o and 58o indicate the presence of the Mo_2FeB_2 tiny nanocrystals already in the as-quenched state. The principal crystallization phase, i.e. bcc Fe(Mo) appears at T_{x1}. Structural transformation from bcc into fcc arrangement is identified at T_{x2}. Later on (at about 690 oC), the crystallization is already well developed.

Differences between both surfaces of the inspected ribbons are also discussed.

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ROCKING CURVE IMAGING AND SYNCHROTRON RADIATION COMPUTED LAMINOGRAPHY AS WIDE PARALLEL-BEAM IMAGING METHODS WITH HIGH SPATIAL RESOLUTION

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We present basis as well as recent advances of two new imaging methods we have developed over the last at about 7 years. The use of intense monochromatic synchrotron radiation (SR) beam and a good 2D detector makes it possible to achieve spatial resolution of parallel beam structure downto a micrometre range. Rocking curve imaging (also called SR area diffractometry) maps local lattice misorientations in crystalline materials from reconstruction of diffraction data, while SR computed laminography (SRCL) reconstructs interior of flat objects from absorption data.

Synchrotron radiation diffraction rocking curve imaging (RCI) technique combines digital X-ray topography (by means of a 2D detector) and conventional Bragg-diffraction rocking curve recording. The method has been developed for local lattice and structure quality control of semiconductor wafers and overgrown structures with spatial resolution downto one micrometer over an extended sample area. Application of this method has been pushed from qualitative wafer structure characterization towards quantitative mapping of local crystalline misorientations and dislocation density and towards one-micrometer spatial resolution to study crystalline morphology of overgrown patterned structures.

Growth of compound materials in ingots, like SiC, GaAs, GaN, InP, leads to inherited imperfections. Regions of specific misoriented macrodefects and dislocation regions in ingots can be qualitatively mapped by RCI and local lattice misorientation angles can be reconstructed. Epitaxial lateral overgrowth (ELO) is an innovative crystal growth technique expected to achieve a better crystal quality. The overgrown layer shows significantly lower density of threading dislocations than in the wetting layer. With micrometer-resolved 2D detector, the RCI allows to monitor the lattice quality and lattice tilts in individual periods of the structure. Significant information can be obtained from individual sample areas as small as 2 micrometers in all three spatial dimensions, and to correct the findings of double-crystal diffraction rocking curve measurements.

Synchrotron-radiation computed laminography (SRCL) is developed and implemented as a method for three-dimensional (3D) imaging of flat and laterally extended devices such as sensors, flip-chip devices and other microsystems. It is based on the acquisition of a series of two-dimensional projections of the device under rotation around an axis which is inclined with respect to the incident x-ray beam by a defined angle 90°. SRCL can be considered as a technique complementary to computed tomography (CT, = 90°) preserving the integrity of laterally extended devices since samples volumes smaller than the field of view have not to be extracted (e.g. by cutting): for planar substrates which are aligned roughly perpendicular to the rotation axis, the integral x-ray transmission on the 2D detector does not change significantly during device rotation. In comparison to CT, this alleviates the presence of imaging artefacts due to missing information in projections where the integral transmission would tend to zero.

The potential of SRCL for inspection of microelectronic devices was illustrated by study of several microelectronic devices such as bonded device or detector chip. For example, after a flip-chip bonding of the device, the flip-chip solder joints are not accessible by visual inspection, while the laminography reconstruction allows to visualize a 3D rendition of bump bonds. This allows to detect voids in the interior of the bump bonds. Such voids affect the long-term reliability of the device when it is exposed to heating/cooling cycles, e.g. due to device operation. Some solid-state electronic devices such as detectors can be studied by both RCI and SRCL methods.