

NEWSLETTER 06 | NOVEMBER 2012

Editorial

While we look ahead with excitement as both the German and the Swedish newly funded research projects unfold, we would also like to take this opportunity to invite you on a journey into the past. DORIS III, DESY's first storage ring, entered "her" well deserved retirement after 43 years of service to the scientific community. DORIS (deriving its attractive name from the term "Doppel-Ring-Speicher") is passing over to the next generation.

Back in the present, we provide updates on some of the German research projects, introduce two members of the Röntgen-Ångström-Cluster Steering Committee and last but not least, share the OTHER news.

Don't forget to visit us online at www.rontgen-angstrom.eu to check on any news in the meantime. Happy Reading!

The editors

NEWS

GERMAN PROJECTS APPROVED

This newsletter introduces four of the eleven German projects approved for funding in the context of the Röntgen-Ångström-Cluster. Please see section "People & Projects" for more info. More project details are to follow, so please make sure to check our website at www.rontgen-angstrom.eu for new information.

UPCOMING CALL

Germany and Sweden are currently coordinating a new call. The details will be announced soon. All info related to the call can be retrieved at www.rontgen-angstrom.eu in due course.

STEERING COMMITTEE MEETING ON SEPT. 26[™]

The 5th Röntgen-Ångström-Cluster Steering Committee meeting took place in Frankfurt/Main on September 26th, 2012. ctromagnetic fields accelerate the electrons in the superconducting resonators © DESY

NEWS

DORIS III - LIGHTS WENT OUT IN OCTOBER 2012

An extraordinary time comes to an end: The second ring accelerator and the first storage ring of DESY's DORIS was switched off on Oct. 22nd. To quote a few figures: DORIS was built from 1969 to 1974 and was initially intended as electron-positron storage ring. The circumference of DORIS is nearly 300 meters. For the first time, collision-experiments of electrons and their antiparticles with energies of 3.5 gigaelectronvolts (GeV) per beam could be carried out in DORIS. In 1978, the energy of the beams was increased to 5 GeV. DORIS has been in operation both for particle physics and for research with synchrotron radiation until 1992.

In 1975, "excited charmonium states" were detected for the first time at DORIS - a discovery that gave birth to the study of the physics of heavy quarks. In 1987, physicists at DORIS discovered that particles called B mesons can transform into their antiparticles, at a surprisingly high rate.

In 1984, two technical innovations were introduced at DESY's Hamburg Synchrotron Radiation Laboratory HASYLAB: "wigglers" and "undulators". These special magnets, that generate particularly high intensive synchrotron light, were installed in large numbers into the DORIS-storage ring. In 1991 the reconstruction of DORIS was complete. For more than two decades DORIS was one of the five strongest sources of the world and at the same time the most powerful X-ray Source of Europe.



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PEOPLE & PROJECTS

GERMAN PROJECTS - PART I

Development of polarized neutron time-of-flight spectroscopy



Project coordinator: Dr. Margarita Russina, Institute of Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin (HZB) **Project:** Spin is a fundamental property of neutrons. Neutron scattering with polarized neutrons has been used in fundamental and condensed matter physics even though the polarization causes a large reduction in flux. In the past polarized

neutron methods were mostly used to separate nuclear and incoherent scattering effects from the magnetic ones to investigate magnetic structures or excitations. They work for a large range of magnetic materials like ferro- and antiferromagnets, spin glasses, spin ices and molecular magnets which are all of fundamental importance. The technique also enables us to identify magnetic moment directions and distinguish chiral magnetic structures.

It was also proposed to use polarized neutron scattering as a substitute for the contrast variation techniques where the spin dependent scattering length can be varied in a similar way as it is done by isotopic substitution that sometimes can be very costly. Such techniques allow us to identify structural correlations, selectively mark parts of the sample or separate coherent from incoherent processes in the same sample without isotopic substitution. These techniques have high potential in applications across chemistry, materials science, physics and even biological materials. The goal of this proposal is the development and implementation of polarization techniques on the time-of-flight spectrometer (TOF) NEAT at HZB. The cold neutron time-of-flight spectrometer NEAT is the key instrument of the neutron instrument suite at HZB to study the dynamics and structure on a very broad frequency range (10 μ eV -150meV) and on a length scale from 0.5 to 100 Å. Currently the instrument is undergoing a major upgrade which

will result in 40 fold increase of sensitivity in addition to the obtained increase of cold neutron flux of the Research Reactor BER II in Berlin.



The large intensity gain provided by the upgrade of NEAT will allow us to implement neutron polarization and polarization analysis and obtain polarized neutron results with advantageous intensities and signal to noise comparable to unpolarized work in the past on this instrument. The experience obtained in the proposed project will be most valuable for highest intensity wide angle TOF spectrometers at European Spallation Source (ESS). Furthermore, the results from this work will be of great use for other wide angle neutron scattering instruments such as diffraction and indirect geometry spectrometers.

Investigations of martensitic transformations under external load by means of in-situ high-energy synchrotron X-ray diffraction



Project coordinator: Prof. Dr.-Ing. Jürgen Eckert, Professor of Materials Synthesis and Analytics at the Institute of Materials Science at Technische Universität Dresden **Project:** This is a collaborative research project of the scientists from the Technische Universität Dresden (Prof. Dr. Jürgen Eckert), Uppsala University (Prof. Dr. Kristina Edström) and Stockholm University

(Prof. Dr. Gunnar Svensson and Prof. Dr. Ulrich Häussermann) within the framework of the German-Swedish cooperation in the field of structural biology and materials science using neutrons and synchrotron radiation. The scientific objective of the project is the investigation of the relations between mechanical properties and the structure of martensitic phases in solids, such as for example nanocrystalline CuZr- and NiTibased alloys, upon compressive or tensile stress and heating. For this, an experimental setup for in-situ X-ray diffraction investigations of the structural changes under load at different temperatures using high-energy synchrotron radiation at the PETRA III storage ring (DESY, Hamburg) will be developed and implemented. The new testing device is not only to be applied for the fulfilment of the current project. It is expected to be used at PETRA III in the future by other researchers investigating phase transformations upon mechanical stress and/or temperature impact.

The participating German and Swedish research groups have experience in materials synthesis and characterization of mechanical and structural properties, including high-energy synchrotron X-ray diffraction. Their expertise will be in demand at all stages of the project beginning with the development of criteria to the new setup, its critical evaluation, and later, by interpretation of the experimental data. (Text: Dr. Ivan Kaban)

Biolubrication of joints: Structural causes of high functionality



Project coordinator: Prof. Dr. Regine Willumeit, Head of Department "Structure Research on Macromolecules" at Helmholtz-Zentrum Geesthacht

Project: The smooth motion of our joints is based on the complex interplay between cartilage, which is a highly specialized nanostructured tissue, and the lubricating

ability of self-assembly structures formed by the molecules of the synovial fluid. It results in friction coefficients which are the lowest found in nature (0.001 - 0.01) and which are difficult to reach in technical processes. The molecular components of the synovial fluid are largely known, and include water, hyaluronic acid, lipids, proteins and glycoproteins. They self-assemble and form a thin lubrication film on the cartilage. However, there is no clear picture of how the molecules interact and how they and the structures they form generate the nearly frictionless movement of joints under load and rapidly changing shear conditions.

In the framework of this project together with our Swedish partners from the Kungliga Tekninska Högskolan (KTH) in Stockholm (Professors Claesson, Dedinaite and Bergström) we aim to build sample environments for two types of measurements. The first intends to exploit the specific nano beam geometry available at the nano focus set up of the MINAXS beamline (Micro and nano focus X-ray Scattering) at PETRA III to perform SAXS and GISAXS measurements under load and shear. This should provide structural information on the molecular organisation with high spatial and temporal resolution. In a second set up we aim to explore the molecular organisation under load and shear on cartilage or implant materials. An increased understanding of the biolubrication of joints also offers potential in other areas, such as development of biomimetic aqueous lubrication systems and design of implant materials that stimulate formation of lubricating self-assembly structures on their surfaces.

ANNOUNCEMENT

Third German-Swedish Workshop

The third German-Swedish workshop within the RöntgenÅngström-Cluster is taking place at the DESY research centre in Hamburg March 18-19, 2013. The workshop focuses on in situ method development for materials science with neutron and synchrotron radiation. More details will be posted on our website www.rontgen-angstrom.eu at the end of 2012.

Advanced factor analysis for Poisson-distributed data



Project coordinators: Dr. Gerald Falkenberg and Dr. Gerd Wellenreuther, DESY, and Prof. Dr.-Ing. Christian Bauckhage (photo), Fraunhofer Institute for Intelligent Analysis and Information Systems IAIS

Project: Currently, imaging data obtained e.g. by scanning X-ray fluorescence (XRF) is usually visualized on the basis of distri-

bution maps representing individual chemical elements (sulphur, iron, and others). In complex samples, e.g. biological systems, most elements are correlated - it would be desirable to rather deal with maps of certain meaningful chemical compositions.

This project consequently tries to develop new approaches based upon factor analysis algorithms, especially those related to non-negative matrix approximation (NNMA). Compared to other factor analysis methods, e.g. principal component analysis (PCA), NNMA enforces non-negativity of the individual factors, which is especially helpful when dealing with nonnegative quantities like photons or concentrations.

New NNMA-algorithms will be developed by the Fraunhofer institute IAIS in St. Augustin, while their evaluation will be done at DESY, e.g. at the Hard X-ray Micro-/Nano-Probe Po6 at PETRA III by scientists both from DESY and MaxLab / University of Lund. We will make these algorithms available to the scientific community as a graphical user interface through the plugin-mechanism for the free XRF-evaluation software PyMca, and also explore their application to other data like e.g. X-ray diffraction (XRD) or combined XRF / XRD.

WORKSHOP

Second Swedish German Workshop within the Röntgen-Ångström-Cluster on Special Topics in Materials Science

During two days (August 28-29, 2012), 9 German and 16 Swedish participants exchanged experiences about special topics of materials science in the context of the Röntgen-Ångström-Cluster. The workshop at Stockholm University was second in a series and followed up on the first workshop held in Göttingen (November 2011). The goals of the workshop included:

- information on upcoming funding opportunities
- presentation of experimental opportunities at the facilities which the Röntgen-Ångström-Cluster focuses on
- realization of an educational program for students/young scientists

The next workshop is planned for March 2013.

PEOPLE

Rolf Greve: Building bridges across academic disciplines

Mats Johnsson: Promoting International Research Infrastructures



Promoting research in the city of Hamburg and beyond is Rolf Greve's mission. He works for Hamburgs Ministry of Science and Research and has been a member of the Röntgen-Ångström-Cluster Steering Committee since it first started. To him, the Röntgen-Ångström-Cluster represents a continuation and expansion of the scientific cooperation of the Northern federal

states that has been evolving over some time. The states of Hamburg, Schleswig-Holstein, Lower Saxony, Berlin, Mecklenburg-Vorpommern and North Rhine-Westphalia have joined forces in the interest of science and research. Rolf Greve sees it as one of his main responsibilities as a member of the Röntgen-Ångström-Cluster Steering Committee to represent the interests of these states.

Greve stresses that it is not enough, "to exchange views pro forma". "Money needs to be invested" to support the communication between scientists in very practical ways by means of conferences, workshops and other information campaigns.

"The scientists within individual disciplines talk to each other regularly. The challenge is to increase the flow of communication between researchers of different disciplines. The added value is achieved by building bridges across various disciplines - for example from physics to chemistry to biology to medicine." This, says Greve, combined with the most up to date facilities at the large research institutes in the Northern region would guarantuee success in research, such as the development of medical remedies.

According to Greve, the wide range of opportunities offered in the context of the Röntgen-Ångström-Cluster across national borders should be made more transparent. Not only largescale equipment but the planned European Spallation Source (ESS) in Lund as well point to numerous possibilities for the scientists in the field of neutron research. New paths will be opened up and establish the north as "one of the leading sustainable innovation regions of Europe", predicts Greve.

MORE NEWS ONLINE

Please check our website regularly. In due course, we will introduce the remaining seven German projects approved for funding in the context of the Röntgen-Ångström-Cluster. www.rontgen-angstrom.eu

IMPRINT

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As a member of the Röntgen-Ångström-Cluster Steering Committee, Mats Johnsson represents the views and interests of the Swedish government. He is senior advisor at the Swedish Ministry of Education and Research responsible for research policies for natural sciences and engineering and for policy and planning. A large part of his work over the past years has been to realize

the government's plans to join and initiate major research infrastructures.

"The Swedish government has several large infrastructures in the pipeline", explains Mats Johnsson. Two of these, the European Spallation Source (ESS) and the Max IV-synchrotron are to be built in Lund. ESS is a European project. Max IV is a national facility open for scientists from all countries budgeted to about 200 million Euro. Another facility, the SciLifeLab in Stockholm and Uppsala is a facility for large scale gene and protein analyses built as a national facility but naturally open for scientists from other countries. SciLifeLab was formed in 2009 and is now in the upscale phase to full size with a yearly budget of about 100 million Euro.

"The Röntgen-Ångström-Cluster and the collaboration around ESS have opened up the possibilities for closer collaboration with Germany and the facilities that are under construction there", says Johnsson. The Swedish government contributes to the planned extensions to Petra III in form of a dedicated beamline and research groups working in Hamburg together with German research groups. "The hope of the Swedish government is to have closer ties between the German large-scale facilities in Hamburg and in Berlin and the facilities in Lund (ESS and MaxLab) and in Stockholm (SciLifeLab)" says Johnsson concluding that "the Baltic Sea area is with these research centres a world class region in science".

The OTHER News



The Swedish Football Miracle

The contribution of sciences to the evolution of mankind is appreciated. We have just applauded this year's Nobel Prize Winners and demonstrated gratitude and respect. Where would we stand today if it wasn't for the continuous progress on the part of scientists and inventors?

However, the glorious moments in time are those that remain unexplained. Miracles, as some would say. The Swedish football world has just been blessed with one: 4 - 4 against Germany. Those who watched the recent World Cup qualifier in Berlin will tell their children and grandchildren how the Swedish team fought back in 30 minutes from 0 - 4 down to a draw. Germany's national football coach, Joachim Löw, will undoubtedly start a scientific investigation into why his team could let a 4 - 0 lead slip out of its hands. He might find some answers. But the truth remains: in football, miracles can happen.