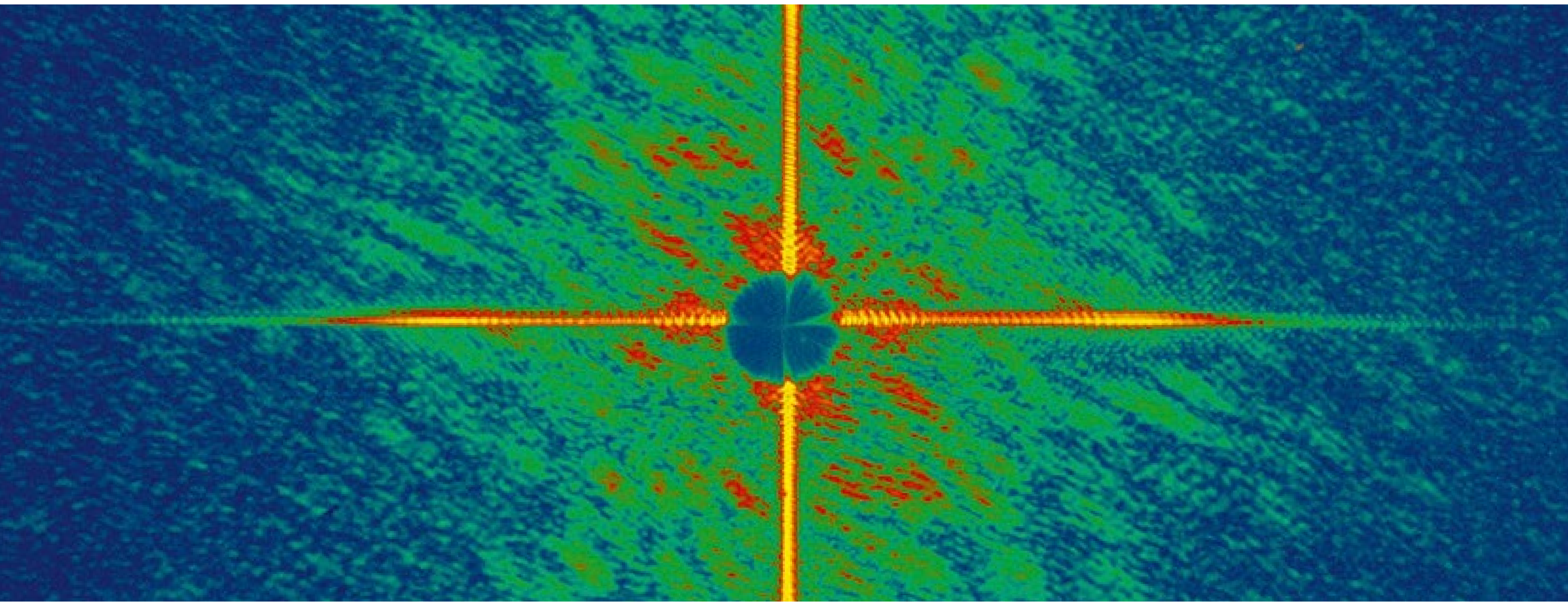
Röntgen
Ångström
Cluster

PROJECTS & PARTNERS – A PORTRAIT

The Röntgen-Ångström-Cluster as a successful German-Swedish Cooperation to strengthen research with synchrotron radiation and neutrons



Vetenskapsrådet

GEFÖRDERT VOM

Bundesministerium für Bildung und Forschung

Welcome! Välkommen! Willkommen!

Partners and Profile

Projects and Participants

Photo: Birgitta Schoch

WELCOME

WILLKOMMEN VÄLKOMMEN

An Interview with the Swedish Head of Delegation and the former German Head of Delegation

Dr. Ralph Dieter, German Ministry for Education and Research (left) and Prof. Ulf Karlsson, Royal Institute of Technology Stockholm

Anders Jonas Ångström and Wilhelm Conrad Röntgen made their discoveries in the fields of spectroscopy and X-rays in the 19th century. They did not know which possibilities for today's scientists they would open up: completely new fields of research are now a reality. To their successors, an immense spectrum of research infrastructures is available in Europe, in particular in Germany and Sweden. The vicinity of these infrastructures as well as universities of both countries naturally suggests a fruitful collaboration.

Today the "Röntgen-Ångström-Cluster" (RÅC) is named after these two research pioneers – a German-Swedish collaboration promoting research with neutrons and synchrotron radiation in the areas of materials science and structural biology. It was initiated in 2009 by the German Federal Ministry of Education and Research and the Swedish government with the aim to expand bilateral cooperation. Since the start of the cluster more than 20 collaborative projects were funded consisting of over 50 partners from both countries.

This brochure presents the cooperation. It illustrates the involved neutron and photon sources and portrays the cluster with the help of representative examples of funded projects from the two mentioned research areas. In addition, it provides information about conditions of funding.

To start off, the Heads of Delegation in the Steering Committee of the Röntgen-Ångström-Cluster, Dr. Ralph Dieter (German Federal Ministry of Education and Research) and Prof. Ulf Karlsson (Royal Institute of Technology, Stockholm) address the most important aspects of the Cluster:

WHAT IS THE PURPOSE OF THE RÖNTGEN-ÅNGSTRÖM-CLUSTER?

Dr. Ralph Dieter: The aim of the Röntgen-Ångström-Cluster is to foster cooperation between Sweden and Germany in research using photons and neutrons. The RÅC allows us to intensify research at the outstanding large-scale facilities in Germany and Sweden, for instance, at the European Spallation Source (ESS) currently under construction

Photos: Ralph Dieter/BMBF, Ulf Karlsson/KTH Stockholm, GettyImages

in Lund, at the research neutron reactor FRM II in Garching and at the European X-ray Laser (European XFEL) in Hamburg and Schenefeld. This pushes German-Swedish collaboration to a new level and favours the necessary growth in the photon and neutron science communities in both countries.
Prof. Ulf Karlsson: The advantage of the RÅC stems from its naturally grown structure: it was developed on the basis of established national funding programmes without adding further bureaucratic complexity for the scientists. This makes it easy for us to create new means of support or to advance existing means.

WHY DOES THIS COLLABORATION STAND OUT FROM OTHERS?

Dieter: With the Röntgen-Ångström-Cluster, our political awareness at the governmental level becomes apparent, stating that any future innovation requires basic research. And research is nowadays mainly international. In order to make the best out of the know-how in photon and neutron science, funding such collaborations across borders is becoming more and more important. Here, cooperation in the Röntgen-Ångström-Cluster plays a role model.
Karlsson: Science doesn't know any national borders and it is a great fortune that we have outstanding research infrastructure so close by, within our countries. The possibilities of collaboration in the Cluster are unique – this is shown by the high number of applicants for funding in the framework of the RÅC.

WHAT IS SPECIAL ABOUT THE GERMAN-SWEDISH COLLABORATION?

Dieter: The close relations between Sweden and Germany in trade, politics, culture and science look back on a long history. They rest on common values and are a true role model for other cooperation. Concerning science, we share the same goal to exploit the research infrastructures available in our countries to the maximum benefit for our societies.
Karlsson: In addition, we also have the advantage that excellent research facilities in Germany and Sweden are available at such a short distance. Our cooperation demonstrates on many levels that science benefits from complementary expertise and the wide range of infrastructures.

WHICH ROLE DOES RESEARCH IN THE RÅC PLAY IN THE FUTURE?

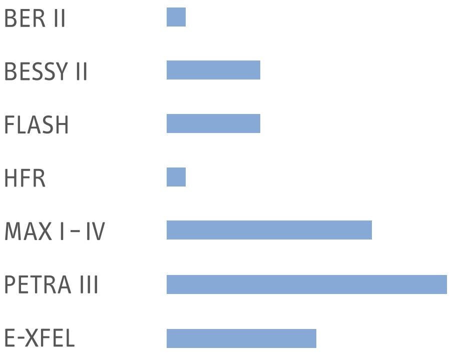
Dieter: Research at photon and neutron sources will remain essential for making advances in materials science and structural biology. The large-scale facilities available to the RÅC provide opportunities and insights into condensed matter that are not available anywhere else.
Karlsson: Results from RÅC-projects will eventually help our societies to find answers to the urgent challenges of our time. For example, how sustainable energy supply and healthy living can be brought about.

WHAT ARE THE ACHIEVEMENTS OF THE RÅC?

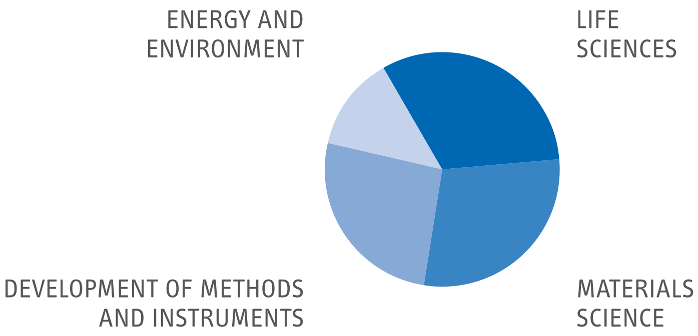
Karlsson: „We have excellent large-scale research infrastructures in Sweden and Germany that perfectly complement each other and therefore act as an incubator for international cooperation. Using the synergies has strengthened the research with photons and neutrons in both countries.
Dieter: In the Röntgen-Ångström-Cluster, we see immediately the benefits of working together across borders. The cluster embodies a handshake, a new quality of fruitful cooperation. Together we have funded more than fifty outstanding research projects so far, as well as the Swedish Beamline at PETRA III, the most brilliant storage-ring X-ray source in the world at the German Electron-Synchrotron DESY in Hamburg. I am absolutely certain, Ångström and Röntgen would be proud of the achievements of the RÅC.

PARTNERS & PROFILE: EXCELLENT GERMAN-SWEDISH RESEARCH & NETWORKING

DISTRIBUTION OF FUNDED PROJECTS



RESEARCH AREA OF THE PROJECTS



Research groups from diverse scientific institutions in Germany and Sweden collaborate under the roof of the Röntgen-Ångström-Cluster (RÅC) with world-leading infrastructures for research with photons and neutrons. In particular, efficiently shared use of these infrastructures in the Baltic region plays a pivotal role. International partners help each other with the design and the construction of new research infrastructures such as, for example, the European XFEL in the Hamburg area and the European Spallation Source ESS in Lund. Another corner stone of the RÅC concerns the stimulation of interest and the support of undergraduate students, PhD students and young scientists. This is realised with the help of activities like summer schools, workshops and many more (for more details see page 11).

Research with photons – generated by storage rings and Free-Electron-Lasers – and with neutrons allows a deep insight into the micro- and nano-cosmos. Due to their short wavelength they are ideally suited as probes to elucidate structures and processes in materials and biological samples – down to the atomic level. With the help of synchrotrons, X-ray lasers and neutron sources it is therefore possible to investigate properties of matter that would not be accessible with the use of conventional laboratory equipment. The most advanced photon and neutron sources in Germany, France and Sweden participate in the Röntgen-Ångström-Cluster. All these facilities offer outstanding possibilities for the German-Swedish collaboration in the area of "condensed matter" with a focus on materials science and structural biology. Scientists who work on topics like new materials or pharmaceutical will be presented with an excellent research environment. These facilities are briefly presented on pages 8 and 9.

NETWORKING IN THE CLUSTER

LUND

MAX IV, MAX IV Laboratory

HAMBURG

E-XFEL

FLASH/DESY

PETRA III/DESY

BERLIN

BER II

BESSY II

GRENOBLE

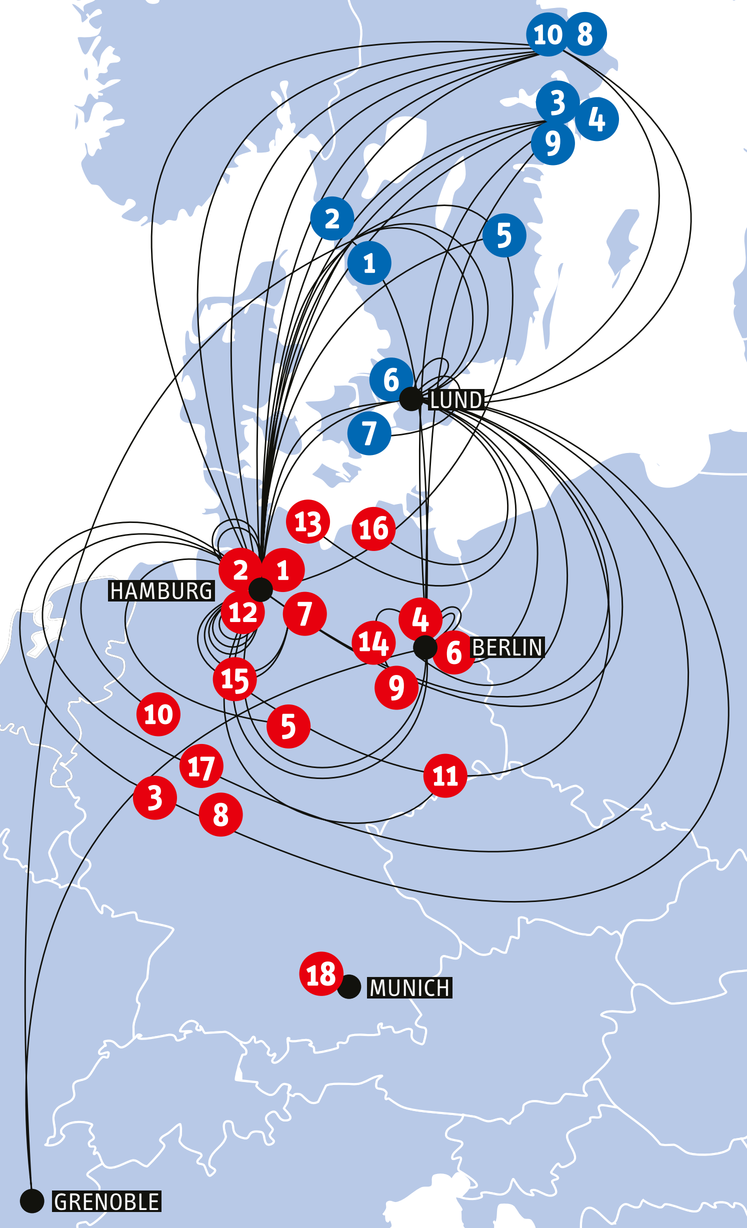
HFR/ILL

MÜNCHEN

FRM II

1. CTH: Chalmers University of Technology
2. GU: University of Gothenburg
3. KI: Karolinska Institute, Stockholm
4. KTH: Royal Institute of Technology
5. LIU: Linköping University
6. LU: Lund University
7. MAH: Malmö University
8. SLU: Swedish University of Agriculture, Uppsala
9. SU: Stockholm University
10. UU: Uppsala University

1. DESY: Deutsches Elektronen-Synchrotron
2. EMBL: European Molecular Biology Laboratory
3. FhG: Fraunhofer-Institute for Intelligent Analysis- and Information Systems (IAIS)
4. FUB: Free University of Berlin
5. GAUG: Georg-August-University of Göttingen
6. HZB: Helmholtz-Centre Berlin
7. HZG: Helmholtz-Centre Geesthacht
8. JLUG: Julius-Liebig-University Gießen
9. MPIKG: Max-Planck-Institute for Colloids- and Interfaces, Potsdam
10. RUB: Ruhr-University Bochum
11. TUD: Technical University Dresden
12. UH: University of Hamburg
13. UL: University of Lübeck
14. UP: University of Potsdam
15. UPA: University of Paderborn
16. UR: University of Rostock
17. US: University of Siegen
18. TUM: Technical University of Munich



This map illustrates how research infrastructures involved in the Cluster are linked to universities and research centres in Germany ● and Sweden ● through collaborative projects. ● denotes cities with large-scale research infrastructures.

BESSY II – THE SYNCHROTRON RADIATION SOURCE IN BERLIN

The storage ring BESSY II at the Helmholtz-Centre Berlin offers synchrotron radiation over a broad energy range with a focus on soft X-rays at about 2,000 electron Volt or below. There are 47 beamlines available to the users to perform experiments in the area of energy research, new materials and life sciences.

EUROPEAN XFEL – THE X-RAY LASER IN HAMBURG AND SCHENEFELD

The European XFEL is a record-breaking Free-Electron-Laser. It will soon deliver ultrashort, hard X-ray pulses – with a 10,000 times higher average brilliance compared to conventional synchrotron radiation sources. This allows not only the structure determination of materials and biomolecules but also “shooting movies” of chemical reactions. The 3.4 kilometre long facility will start operation in 2017.

FLASH – THE UV- AND X-RAY LASER IN HAMBURG

FLASH has been the first Free-Electron-Laser worldwide to produce ultrashort light pulses in the UV and soft X-ray range, being complementary to the energy range available at the European XFEL. FLASH is a pioneering facility at the Deutsche Elektronen-Synchrotron DESY in Hamburg and since 2005 delivers laser-like flashes of light. About 250 scientists per year perform experiments at the beamlines in operation so far. The extension FLASH II offers an additional laser source with up to six experimental stations being available in the future.

MAX IV – THE SYNCHROTRON RADIATION SOURCE IN LUND

MAX IV currently delivers the best collimated X-rays in Europe, a quality that is essential for various techniques. At the heart of the facility are two storage rings, a smaller ring for UV and soft X-rays and a larger ring for hard X-rays. This facility of the latest generation will provide 14 beamlines for about 2,000 users per year. MAX IV in Lund, southern Sweden, was inaugurated in June 2016.

PETRA III – THE SYNCHROTRON RADIATION SOURCE IN HAMBURG

PETRA III at the Deutsche Elektronen-Synchrotron DESY in Hamburg is currently the most brilliant source for hard X-rays in the world. Especially those users who need to penetrate deep into the material or investigate very small samples benefit from the high photon intensity. About 2,000 users perform experiments at the 14 operating beamlines. In September 2016, two new experimental halls were inaugurated which will offer up to 11 new beamlines, one of which is the Swedish beamline for high-energy materials science.

Photos: HZB/Euroluftbild.de, European XFEL, DESY 2015/Dirk Nölle, Universität Lund, DESY

BER II – THE RESEARCH NEUTRON SOURCE IN BERLIN

The research neutron source BER II at the Helmholtz-Centre Berlin (HZB) delivers neutrons for a broad spectrum of scientific investigations, in particular materials science. A total of 10 modern instruments for thermal or cold neutrons are available to external users. In addition, BER II provides sample environments for matter under extreme conditions, including high or very low temperatures, high pressure and high magnetic fields.

ESS – THE SPALLATION SOURCE IN LUND

The European Spallation Source ESS is currently under construction in Lund and will set new standards for research with neutrons: the facility will deliver neutrons with the highest intensity worldwide and will enable scientists to perform experiments never done before in materials research and life sciences. A total of 22 instruments are planned which will gradually be commissioned until 2025, with first neutrons for seven instruments being expected in 2019.

FRM II – THE RESEARCH NEUTRON SOURCE IN GARCHING

The neutron source FRM II of the Technical University of Munich offers the worldwide highest neutron flux per unit of thermal power produced by the reactor. Users are able to investigate the structure and dynamics of materials at a scale of 0.1 nanometres up to micrometres with a broad range of neutron energies. At the 27 instruments, they conduct around 700 experiments per year in many different disciplines.

ILL – THE RESEARCH NEUTRON SOURCE IN GRENOBLE

The Institut Laue-Langevin is currently the source with the highest flux of neutrons in the world. The reactor delivers a broad energy range from very cold to thermal neutrons for about 40 instruments which allow experiments under extreme conditions of the investigated samples. Up to 1,500 users visit the ILL every year to determine structural and dynamic properties of materials or biological samples.

Photos: Bernhard Ludewig, ESS, Bernhard Ludewig, ILL/Jean-Luc Baudet

PROMOTING JUNIOR SCIENTISTS IN THE CLUSTER

From the outset, one of the aims of the RÅC is the promotion of junior scientists. The hunger for knowledge and enthusiasm for experimentation of young researchers always shows to be contagious among all participants. Summer schools, workshops and meetings with young people provide, as shown time and again, valuable contacts and experiences, problems and solutions, bright ideas and challenges.

Next to single workshops or workshop series, there are two attractive schools in which young academics gain qualifications and get in contact with peers.

The annual **RACIRI summer school** represents a common initiative of Sweden, Russia and Germany within the international research cooperation of the Röntgen-Ångström-Cluster (**RÅC**) and the Ioffe-Röntgen-Institute (**IRI**). Each summer school features a scientific lead topic from the field of materials research and is dedicated to a specific aspect of how to best exploit large-scale facilities. Up to 80 scientists at the junior level can participate in this school.

The practice oriented **MATRAC summer school** has been conceived as an international workshop with the aim to provide an overview of how to make best use of neutrons and synchrotron radiation with regards to **materials science** in the **RÅC**. The school takes place twice a year and offers the participants the possibility to expand their competence at research infrastructures. The intended audience of MATRAC are about 40 European students and young scientists.

In the RACIRI summer school, junior researchers have the chance to network, to broaden their horizon and to look beyond their own field of activities.

"An absolute highlight for us junior researchers was the keynote lecture from the Nobel Laureate Ada Yonath at **RACIRI**."

Sebastian Ekeroth
PhD student, Linköping University, Sweden

"I'm certain the practical knowledge I acquired at **MATRAC** about international cooperation will play an important role in my future research."

Milad Gademi Yazdi
PhD student, Lund University, Sweden

"The workshops are a great opportunity to create networks and to learn in a systematic way."

Fang Liu
Assistant Professor, Chalmers University of Technology, Gothenburg, Sweden

Photo: Marta Mayer, DESY, GettyImages

THE **FUNDING**

… by the German Federal Ministry for Education and Research and by the Swedish Research Council in the framework of the Röntgen-Ångström-Cluster addresses German and Swedish researchers. Their expertise and method competence fruitfully complement each other in research collaborations.

The intense binational exchange among research groups is expected to prove beneficial to the establishment of long-term scientific-technical collaborations at large-scale facilities of the two countries. At the centre of the funding is the continuous development of methods and instruments and thereby, an increase in the performance of existing or future large-scale facilities for neutron and synchrotron radiation in the region.

INFORMATION FOR APPLICANTS

Interested researchers can apply for national funding within the framework of the Röntgen-Ångström-Cluster in Germany or in Sweden, respectively, on the basis of a common call. A prerequisite is cooperation between at least one partner from each of the two countries. In Germany, all higher education institutions may participate in the Cluster and under certain conditions also research institutions which are co-funded by the federal state and single states. In Sweden, individual researchers can send applications to the Swedish Research Council if they are linked to a Swedish administrating organization and if they serve as project leaders and scientific supervisors in the research funded by the Swedish Research Council.

A collaborative activity is supposed to last between three and four years and to be regulated by a cooperation agreement between the partners.

Apart from funding research projects over a period of several years (totalling 37.4 million € so far), additional activities are funded to improve the establishment of long-term networks between German and Swedish research groups. Funding of networking activities may be used for visiting researchers, workshops or jointly organised conferences. In addition, education of highly motivated and qualified junior scientists within the framework of teaching activities, such as summer schools, is supported by the networking activities. The funding is currently coordinated in Sweden by the Swedish Research Council and in Germany by the project management agency Projektträger DESY on behalf of the German Federal Ministry for Education and Research.

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PROJECTS & PARTICIPANTS: SOME PROJECTS OF THE RÖNTGEN-ÅNGSTRÖM-CLUSTER WILL BE PRESENTED ON THE FOLLOWING FACE TO FACE PAGES. THESE PROJECTS GIVE AN OVERVIEW OF THE DIVERSITY OF THE SOCIAL CHALLENGES THAT ARE ADDRESSED BY RESEARCH WITH PHOTONS AND NEUTRONS.

UNDERSTANDING CATALYSIS: RESEARCH FOR A SUSTAINABLE USE OF RESOURCES

The social needs for energy efficient and sustainable technologies are growing steadily. New production methods for fuels and chemicals need to be developed to decrease the oil dependency. This is one way how the impact of oil consumption on our environment and society can be reduced. RÅC-research groups from Paderborn and Gothenburg use synchrotron radiation of MAX IV and PETRA III to contribute to the solution of the resource and energy problem.

The process of catalysis (from the Greek word for resolution) plays a central role in today's industrial production, as for example in food and fuel production. Technical solutions employing catalysis will remain essential for the development of sustainable production processes. Often considerable amounts of scarce elements are required in today's catalytic production processes that may be laborious and expensive to obtain. The development of durable catalysts that require only a minimum of precious resources is therefore of considerable importance. It is in this field of research where the collaboration of the Universities of Paderborn in Germany and Chalmers University of Technology in Sweden are active.

THREE APPROACHES TOWARDS SUSTAINABLE FUEL SYNTHESIS

Professor Matthias Bauer (Paderborn) and his Swedish colleague Professor Per-Anders Carlsson (Gothenburg) focus in their project on three challenging catalytic processes which they regard as a promising path towards sustainable fuel synthesis:

"The Swedish-German constellation is unique as it combines complementary experimental and theoretical competences. This is what we need to tackle the challenges regarding novel catalyst preparation and evaluation techniques, ex-situ and in-situ characterisation of materials and computational modelling – different fields that all require significant method development by experts."

Per-Anders Carlsson *Chemistry and Chemical Engineering, Applied Surface Chemistry, Competence Centre for Catalysis at Chalmers University of Technology, Gothenburg, Sweden*
E-mail: per-anders.carlsson@chalmers.se

1) photocatalytic synthesis of hydrogen from water splitting,
2) direct synthesis of methanol from bio-methane and
3) hydrogenation of carbon dioxide to methanol.

The aim of the cooperation is a better understanding of all involved chemical processes as only those mechanisms that are properly understood can be further developed. The researchers approach these challenges by combining novel synchrotron-based methods with theory-based modelling. Their work at MAX IV and PETRA III enables the two scientists to look deeper into the reaction processes. This is done while the processes are taking place, i.e. in-situ and time-resolved. Advanced structure-function correlation experiments on catalysts are performed using X-ray spectroscopy and high-energy X-ray diffraction. They also optimised methods to their needs. Specifically, a new X-ray emission spectrometer and an infrared spectroscopy set-up are created in this project. Results of measurements with these new instruments are then combined with computer simulations to obtain a model of the reaction mechanism. The new instrumentation is therefore paving the way for future in-situ studies in materials science at PETRA III and MAX IV.

FINDINGS ADVANCE A MULTITUDE OF DISCIPLINES

The further development of synchrotron methods with unique possibilities for the study of catalysis has a great influence on disciplines such as biochemistry, materials science and energy research. With the spectrometer developed by Bauer and Carlsson, a unique instrument is available for all users at PETRA III. Regarding energy research, the outstanding possibilities are reinforced by the fact that the experimental infrastructure is specially tailored to work on this topic. Significant progress can therefore be expected in the development of sustainable chemical reactions by investigating them with intense X-rays.

"Several scientific disciplines can benefit from the development of synchrotron methods at the end of the project: biochemistry, catalysis research, energy research, and so on."

Matthias Bauer *research group "Inorganic Chemistry" at the University of Paderborn, Germany*
E-mail: matthias.bauer@upb.de

Photos: xxx, xxx

NANOWIRES IN THE FOCUS: RESEARCH FOR EFFICIENT SOLAR CELLS

Sunlight is a promising renewable energy source, but current solar technologies work rather inefficient. Recent work indicates that nanowires may enhance solar cell efficiency. But how do you investigate these tiny crystals? Research groups from Göttingen and Lund University which are funded in the framework of the RÅC use hard X-rays of PETRA III and MAX IV to develop new characterisation tools.

Solar energy has the potential to supply the world's need for electricity in a clean and renewable manner. One way to harvest solar energy is a solar cell. However, current solar cells are expensive to manufacture and typically convert only 20% to 30% of the incoming solar energy into electricity. A recent approach to solve this problem regards nanowires. These are tiny structures grown vertically on a suitable substrate like corn on a field. They consist of elongated semiconductor crystals, about 10,000 times thinner than a human hair and use only a fraction of the material of planar devices. Moreover, nanowires show a huge potential for the use in light-emitting diodes and transistors.

HIGHEST RESOLUTION FOR SMALLEST NANOSTRUCTURES

Professor Magnus Borgström and his team from Lund University have demonstrated that nanowires can produce as much electricity as thin film solar cells made up from the same material but with far smaller amounts of it per square metre. To further develop these nanowire solar cells it is crucial to have suitable characterisation methods at the scale of a single nanowire but many traditional tools developed for planar electronics work poorly for nanostructures. Professor Tim Salditt and his team from Göttingen University can help at this point; they run an instrument for nano-imaging with X-rays at PETRA III which is perfectly suited for Borgström's desired investigations and offers a resolution of 10 nanometres.

USEFUL FOR MANY TYPES OF NANOMATERIALS

In this project funded in the framework of the RÅC, the German and Swedish scientists collaborate to develop novel X-ray characterisation tools that are tailored to single solar cell nanowires. The researchers benefit from each other's expertise: The Salditt

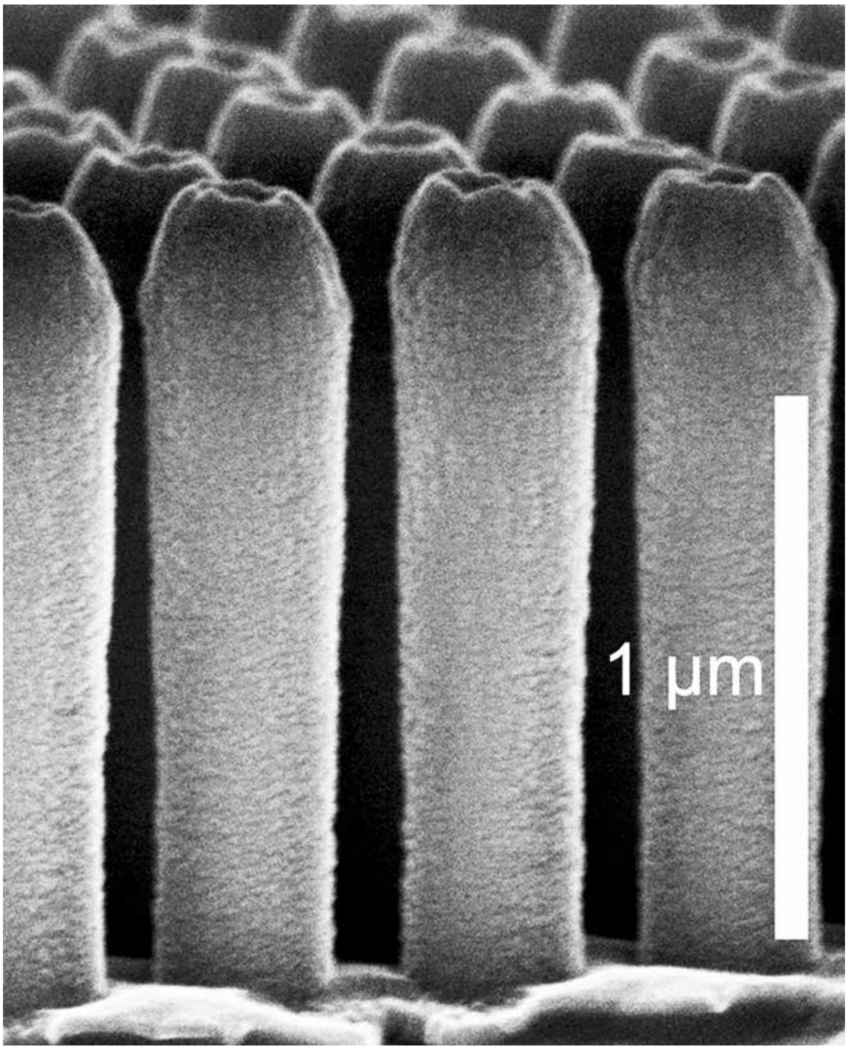
"The main research infrastructure for our project is the storage ring PETRA III. At beamline P10, our project partners from Göttingen have installed a novel X-ray microscope that is particularly suitable for the intended in-operando studies on the nanometre scale."

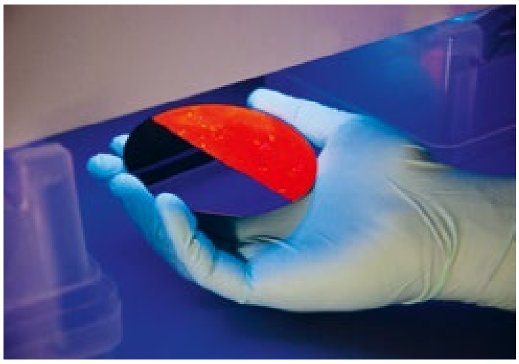
Magnus Borgström *Solid State Physics Department, Lund University, Sweden*
E-mail: magnus.borgstrom@ftf.lth.se

"Thanks to funding in the context of the RÅC, we can extend the sample environment and implement various improvements of the instrument, especially suppressing vibrations of the sample to a large extent."

Tim Salditt *Experimental Physics, Georg-August-University Göttingen, Germany*
E-mail: tsalditt@gwdg.de

group focuses on characterisation methods while the Borgström group is responsible for producing the nanowires. Borgström and Salditt want to image processing layers, doping levels and electric fields in single nanowires. For this purpose, the team develops X-ray imaging and fluorescence methods. Taking advantage of the long penetration depth of hard X-rays, the groups from Göttingen and Lund will develop sample holders and measurement setups to probe individual solar cell nanowires in operation. The developed methods will not only be useful for solar cells, but for many types of nanodevices like quantum dots, phase-change materials, ferroelectrics, perovskites or metal nanostructures.





Like bristles of a toothbrush: This scanning electron microscopic image shows a side view of solar cell nanowires grown on a substrate.

Photos: Magnus Borgström / Universität Lund (2), Georg-August-Universität Göttingen

A VIEW ON MATERIALS ENGINEERING: RESEARCH FOR MODERN MATERIALS

A shared ambition and an effective partnership in combination with a range of complementary skills are at the heart of the scientific success of the RÅC-project of Kristina Edström and Jürgen Eckert. The collective effort of the Swedish and German teams from Uppsala and Stockholm Universities and the Technical University (TU) and Institute for Solid State Research (IWF) in Dresden were geared towards gaining more knowledge about the behaviour of metals and metal alloys under mechanical stress. The aim is to develop new functional materials with advanced mechanical properties.

A fruitful collaboration between the German and Swedish scientists is what Professor Jürgen Eckert describes as one of the most essential outcomes of the research carried out together with his Swedish colleague, Professor Kristina Edström of Uppsala University, along with an impressive result: the setup for in-situ X-ray diffraction studies of metallic, crystalline and amorphous alloys under various conditions at the PETRA III storage ring (Deutsches Elektronen-Synchrotron DESY, Hamburg). According to Eckert, the collaboration was essential for the realisation of the project tasks.

HAND IN HAND

The German side contributed their long-standing experience in the fabrication of bulk metallic glasses and composites and in the characterisation of mechanical properties by laboratory techniques. The Swedish partners added their invaluable experience in materials synthesis and structure characterization by techniques such as electron, neutron and X-ray diffraction. In the case of Edström and Eckert, RÅC opened the doors for this successful collaboration.

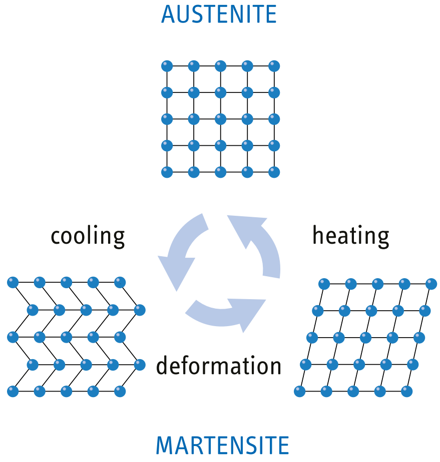
DEVELOPMENT OF NEW COMPOSITE MATERIALS

The developed setup for in-situ X-ray diffraction studies of metallic alloys upon tensile or compressive load and at different temperatures serves as a versatile sample environment. It has been tested at the laboratory in Dresden and is now in user operation at PETRA III. The setup opens new possibilities for materials scientists in their investigations of structure-property relations. In the opinion of the two researchers, the setup further enhances DESY's materials science programme.

The results of the research accomplished by the involved scientists at the numerous locations will help pave the way for the successful development of new materials with advanced properties in the future. The knowledge obtained for copper-zirconium- and nickel-titanium-based alloys in amorphous and crystalline state bring about a better understanding of the relationship between the structure and the mechanical behaviour. It shows possible ways to produce metallic glass matrix composites.

"International cooperation has always been essential for scientific progress, and it becomes much more crucial in times of globalization. Of course, there is a possibility to learn about research of others from publications in scientific journals or conference presentations. But this is not comparable with personal contacts and a joint activity on the same topic, in which the collaborating groups support each other by available knowledge, expertise as well as equipment, as we do in our RÅC-project."

Jürgen Eckert *Formerly IWF Dresden, now Erich Schmid Institute for Materials Science, Austrian Academy of Sciences & Department of Materials Physics, Montanuniversität Leoben, Austria*
E-mail: juergen.eckert@unileoben.ac.at



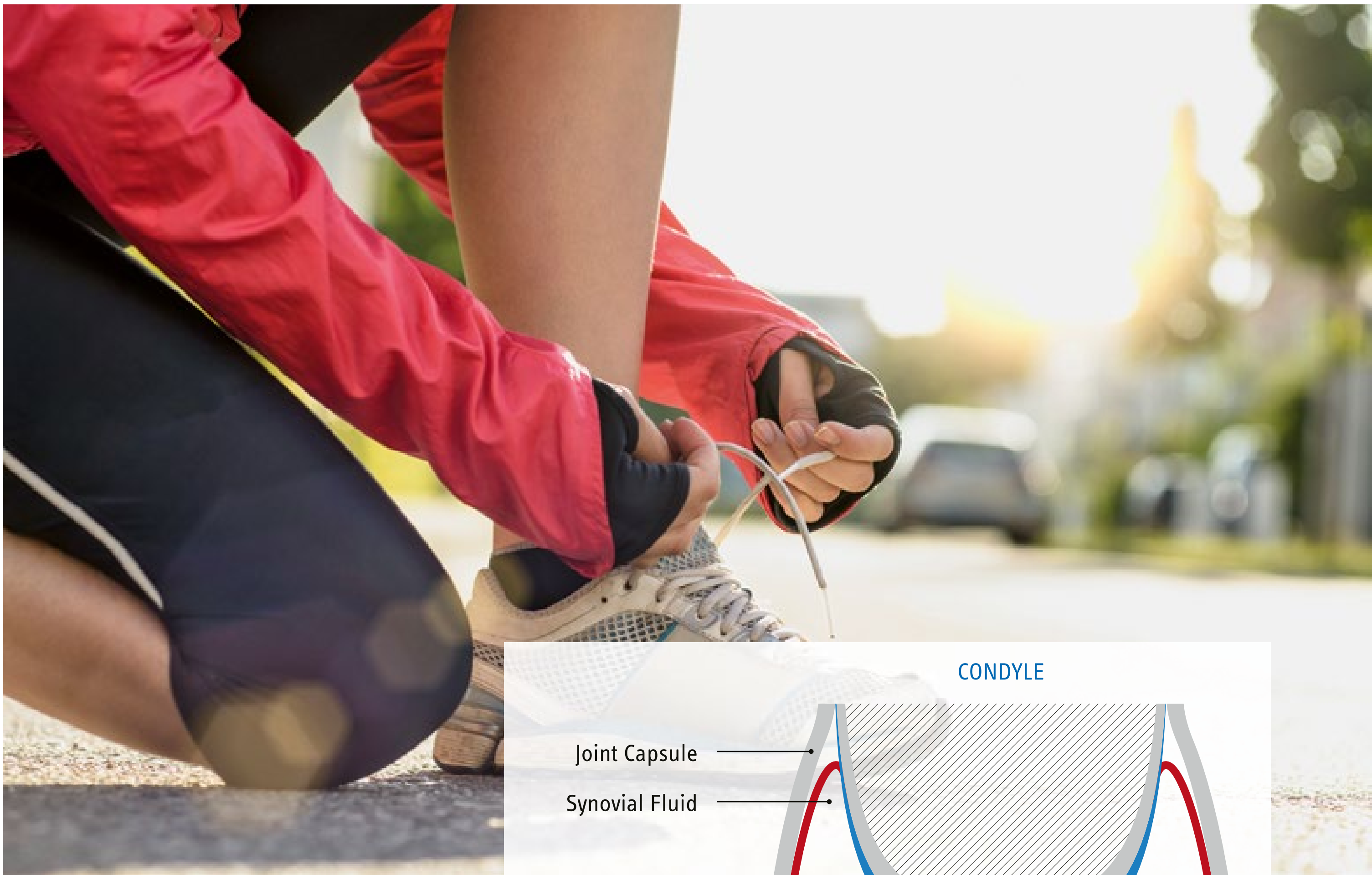
This project investigated, among other questions, how nitinol behaves under tensile and compressive stress. The metallic alloy of nickel and titanium possesses a special property called shape-memory. First a phase transformation takes place upon cooling or shaping, i.e. the crystal lattice changes. Upon heating, the deformation is revoked and the alloy goes back to its original state. The paper-clip on the left was made from nitinol.

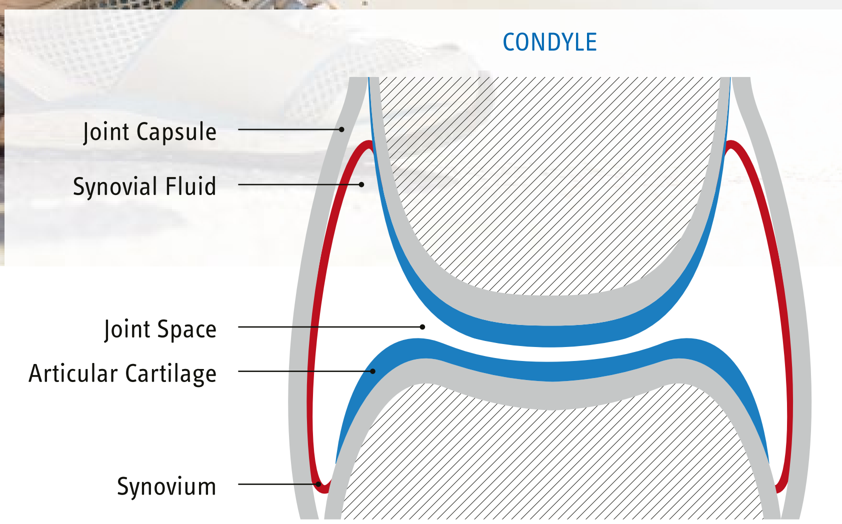
"The instrument we were able to develop together with our German colleagues opened up new possibilities for materials science to investigate the relationship between structure and properties of a material."

Kristina Edström *Professor at the Chemistry Department, Ångström Laboratory, Uppsala University, Sweden*
E-mail: Kristina.Edstrom@kemi.uu.se

LEARNING FROM NATURE:
RESEARCH ON THE SYNOVIAL FLUID

To keep joints moving from the cradle to old age, the joints need lubrication, which is provided by the synovial fluid. While the composition of synovial fluid has been known among researchers for quite some time, there is still a lack of precise knowledge regarding the interaction of components of the synovial fluid. Research groups of the Helmholtz-Centre Geesthacht and KTH Royal Institute of Technology, funded in the framework of the RÅC, used the high pressure rheometer at PETRA III to study samples under various conditions.





The human knee joint is a masterpiece of Nature: With the help of the synovial fluid – investigated in this collaborative project – the components of the knee move almost frictionless along each other. This serves as a model in industrial applications, for example, to improve implant materials.

"There has been a lively scientific exchange between our groups in Germany and Sweden. We were in permanent contact through E-Mail, Skype and mutual visits in Hamburg and Stockholm."

Regine Willumeit-Römer *Division "Metallic Biomaterials", Helmholtz-Centre Geesthacht, Germany*
E-mail: regine.willumeit@hzg.de

The synovial fluid is as efficient as no other fluid in Nature: it results in an almost frictionless movement of cartilage in the joint. For comparison: when steel glides on ice, the coefficient of friction is about ten times higher. How do molecules in the synovial fluid interact under load and rapidly changing shear conditions? What are the structural reasons for high functionality of joint lubrication? A German-Swedish research collaboration of the RÅC got to the bottom of these questions.

INVESTIGATION UNDER HIGH PRESSURE AND SHEAR

In order to investigate the interaction of the synovial-fluid-components Professor Regine Willumeit-Römer and her team from Helmholtz-Centre Geesthacht developed sample environments for two types of measurements. Small-angle X-ray scattering measurements utilizing a microfluidic setup were performed to investigate the behaviour of the different components under very high shear rates. Microfluidics is the science of the behaviour of fluids that are constrained to a sub-millimetre space – this is when laws governing the fluid's behaviour we know from everyday life are breaking down. Furthermore, a sample cell was manufactured which offers the opportunity to do measurements under different load and pressure conditions. In this regard, the high pressure rheometer is unique in the world, available only at PETRA III. The team of Professor Per Martin Claesson focussed on how to achieve low friction in the boundary lubrication regime in aqueous media. According to the two group leaders both science and industry can learn a lot from biolubricants, in particular for biomimetic lubricants and self-assembly structures to achieve low frictional forces and high load bearing capacities.

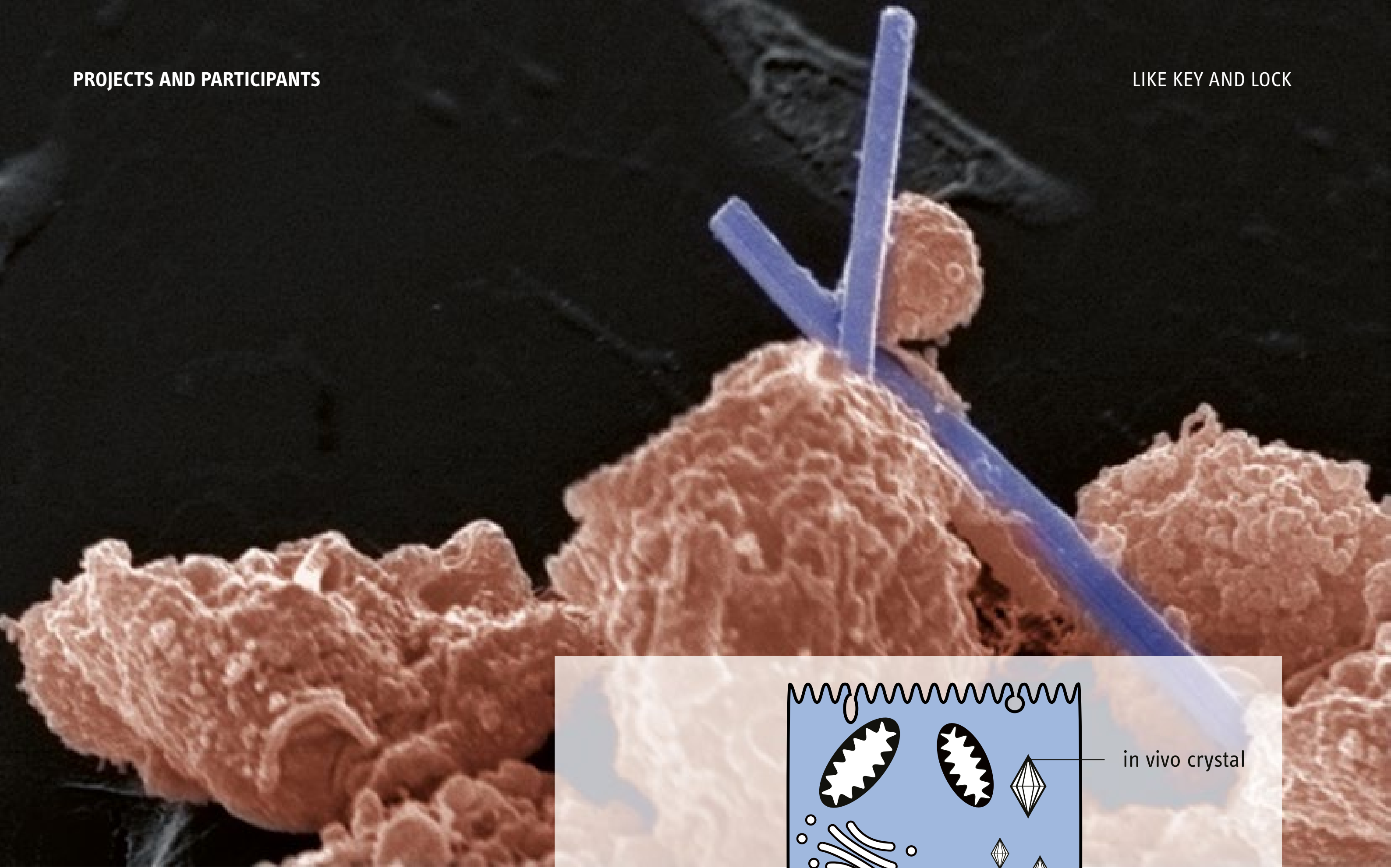
THE LONG-TERM GOAL: TO IMPROVE THE QUALITY OF IMPLANTS

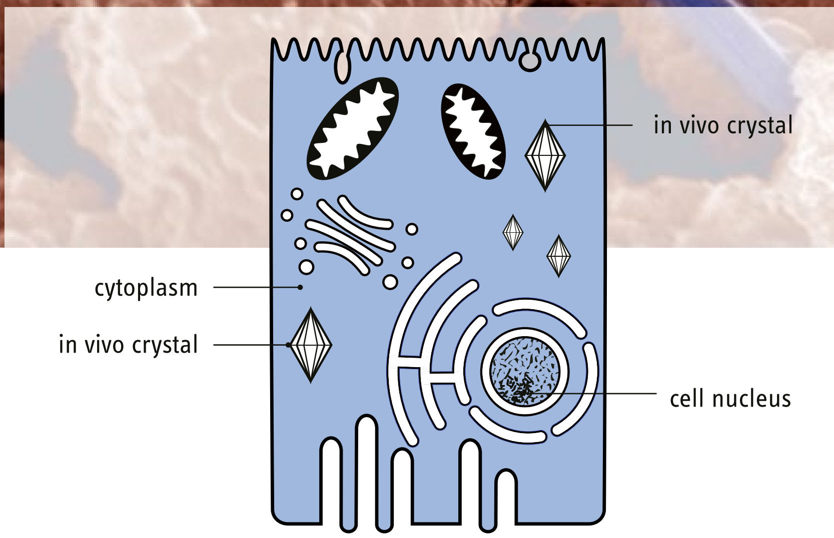
Thanks to the RÅC, both partners have been able to contribute their expertise which has complemented one another outstandingly. The two researchers are convinced that together with further investigations they could help to develop lubricants and surfaces that improve, for example, the quality of implants used in biomedical technology. Especially, the newly developed sample environments will prove very useful for the study of other rheological systems, so that new challenges can be tackled, such as in the field of polymer physics.

"In combination with additional studies, our findings can contribute to the development of lubricants and surfaces. Eventually, they will advance biomedical technology and lead to better quality implants."

Per Martin Claesson *Division of Surface and Corrosion Science, KTH Royal Institute of Technology*
E-mail: percl@kth.se

Illustration: Britta von Heintze, Projektträger DESY | Photos: iStock, Helmholtz-Zentrum Geesthacht, KTH Stockholm





Thanks to the collaboration within the RÅC, the two researchers complemented and deepened their expertise on in-vivo crystallisation – growing crystals in living cells.

LIKE KEY AND LOCK: RESEARCH ON CUSTOM-FIT PHARMACEUTICALS

The fight against a large variety of diseases requires highly selective and efficient drugs. These can be obtained by intelligent design based upon the target molecule's three-dimensional structure which in turn is determined at synchrotrons like PETRA III and MAX IV or in the future at the European XFEL. Large-scale X-ray facilities therefore provide us with valuable information in the area of life sciences.

"Within the RÅC collaboration, we complemented our expertise, in particular regarding the in-vivo crystallisation of proteins. In this way, our joint research activities will be expanded and both of us benefit from the other one's experiences."

Christian Betzel *Institute for Biochemistry and Molecular Biology, University of Hamburg, Germany*
E-mail: Christian.Betzel@uni-hamburg.de

The development of efficient pharmaceuticals often relies on the knowledge of the atomic structure of a target molecule on which the pharmaceutical is meant to perform its medical action. The drug has to fit to the pathogen like a key to the lock. X-ray crystallography is the preferred technique employed in that process, called structure-based drug design, to obtain the atomic structure for many important targets, mainly proteins. For this technique to work, the protein molecules have to be arranged in a crystalline form. This RÅC-project of Professors Christian Betzel, Henry Chapman, Janos Hajdu and Richard Neutze helped to speed up the process by improving a method for crystallising a protein and the instrumentation used to deliver protein crystals to the X-ray beam. Through collaboration in the RÅC, the researchers from Germany and Sweden were able to bundle and expand their expertise on growing crystals in living cells – called in-vivo crystallisation.

A NEW AUTOMATED CRYSTALLISATION PROCEDURE

The research groups exploited the previously discovered possibility to crystallise a target protein inside living insect cells and established an automated procedure to produce and evaluate these microscopic crystals. In a second part of the project, methods and instruments were developed to use these crystals in the most efficient way for collection of crystallographic data at either synchrotron radiation sources or X-ray free-electron lasers. With this combination of improvements it became possible to grow large quantities of crystals from proteins that were not available in crystalline form before and also to determine their structure through a method that is now known as serial in-vivo crystallography. Several techniques were designed and optimised to present the crystals to the highly focussed X-ray beam, such that as many crystals as possible were exploited for collection of diffraction data. These data are then combined and processed with dedicated software to elucidate the three-dimensional protein structure, the starting point for the design of most effective drugs. As a result, this collaboration succeeded in establishing the structure determination from the smallest crystals ever used at a synchrotron radiation source and in paving the way for serial crystallography at room temperature.

"The research infrastructure in Germany and in Sweden – in combination with the respective experts for the facilities – offers scientific possibilities in a geographically small area that is unparalleled in the world. A brilliant basis on which we can work without frictional losses."

Janos Hajdu *Laboratory for Molecular Biophysics, Uppsala University, Sweden*
E-mail: janos@xray.bmc.uu.se

BRIDGING THE GAP BETWEEN MODEL & EXPERIMENT: RESEARCH ON THE STRUCTURE AND DYNAMICS OF PROTEIN

Structural information about macromolecules at the atomic level can best be obtained by X-ray crystallography. This information is essential in understanding protein function and in designing pharmaceuticals. To learn more from macromolecular crystal structures, RÅC research groups from Helmholtz-Centre Berlin and Karolinska Institutet Stockholm gather all available information and provide users with tools to decide whether their protein model is a realistic explanation of the experimental data.

No other technique has contributed more to the detailed understanding at atomic resolution of biological, biochemical and biomedical processes than macromolecular crystallography. Its principle is that the molecules to be studied have to be crystallised: Trillions of molecules (1 trillion = 1.000.000.000.000) have to be assembled in the same orientation into the periodical arrangement of a crystal. This crystal is then exposed to high-intensity X-rays such as those available at synchrotron beamlines. The resulting diffraction patterns are recorded using modern detectors. From those diffraction patterns the underlying three-dimensional structure can be deduced.

FROM STATIC TO DYNAMIC PROPERTIES

Traditionally crystallography is seen as a static technique. However, more and more evidence is accumulating that dynamic aspects of macromolecular structures are also contained in crystallographic data. In this RÅC-project the German and Swedish research groups are trying to push the current limits of crystallography by deducing the dynamic behaviour of the protein from a variety of its structure in different states.

The researchers use the macromolecular crystallography beamlines at the X-ray source BESSY II that are specially designed for highly automated structural analyses of protein crystals. With more than

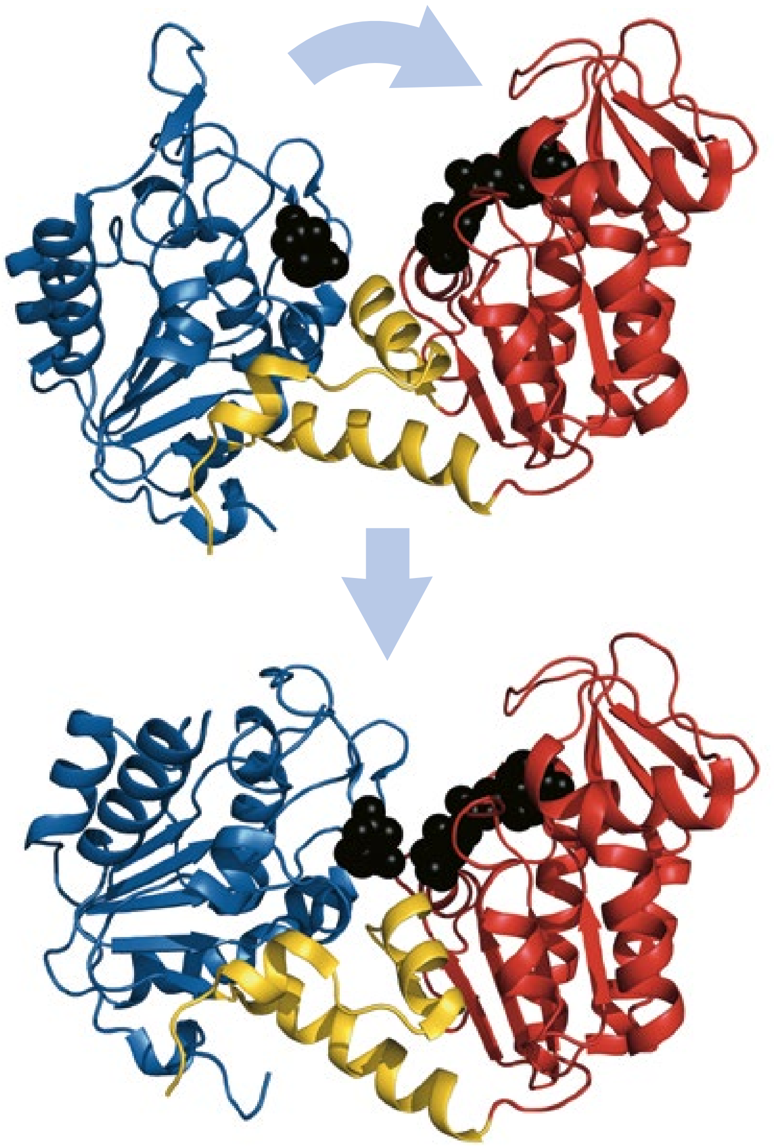
"The Röntgen-Ångström-Cluster allows participating scientists to use large scale facilities jointly and systematically. This offers valuable possibilities. We benefitted from the collaboration with our Swedish colleagues as we were able to use their state-of-the-art software tools. "

Manfred Weiss *Institute for Soft Matter and Functional Materials, Helmholtz-Centre Berlin, Germany*
E-mail: manfred.weiss@helmholtz-berlin.de

2000 solved structures of protein molecules so far, these beamlines are the most productive in Germany. The German group contributes a large amount of experimental data as well as the knowledge to automatically process and evaluate these data. The Swedish group provides knowledge about algorithmic methods and theoretical approaches which is implemented in computer programs. Combining their expertise, the scientists will be able to fully exploit the information about dynamics that is present in macromolecular structures.

THE GOAL: AN IMPROVED AND SUPERIOR MODELLING TOOL

The researchers are convinced that their work will allow bridging the gap between modelling and experiment. Many areas of research could advance: the pharmaceutical industry will benefit from the results since knowledge of the dynamics of the target molecule is very important for designing a medical drug against that target. The results are central to computational crystallography and highly relevant to the whole field of structural biology. The tools may be applicable to other structural biology techniques where dynamics is relevant, like small-angle X-ray scattering and electron microscopy.



The dynamic behaviour of a target protein is of great importance for the design of pharmaceuticals: this protein with flexibility between its blue and red region can bind a medical agent only in the state at the bottom of the picture.

"For the Swedish side it is clear that many interesting cases would not have come under scrutiny were it not for the German collaborator's experimental data. This includes the evaluation of special cases as well as the analysis of data collected systematically under different conditions."

Bernhard Lohkamp *Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm, Sweden*
E-mail: Bernhard.Lohkamp@ki.se20/21

STEERING COMMITTEE
AND CONTACT INFORMATION

The Röntgen-Ångström-Cluster is run by a Steering Committee consisting of seven German and seven Swedish representatives. They meet twice a year.
The Heads of Delegation are currently Ulf Karlsson, Professor at the Royal Institute of Technology (KTH) in Stockholm, for the Swedish side, and until April 2017 Dr. Ralph Dieter of the Federal Ministry of Education and Research (BMBF) in Bonn, on the German side.

REPRESENTING THE GERMAN SIDE

Dr. Ralph Dieter *Federal Ministry of Education and Research, Former Head of Delegation*

Prof. Dr. Helmut Dosch *Deutsches Elektronen-Synchrotron DESY (Hamburg), coordinator*

Prof. Dr. Götz Eckold *University of Göttingen*

Dr. Rolf Greve *Hamburg Federal Ministry for Science and Research*

Prof. Dr. Winfried Hinrichs *University of Greifswald*

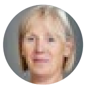
Prof. Dr.-Ing. Anke Rita Kaysser-Pyzalla *Head of Technical University Braunschweig*

Prof. Dr. Lutz Kipp *University of Kiel*

REPRESENTING THE SWEDISH SIDE

Mats Johnsson *Swedish Ministry of Education, Culture and Research*

Prof. Dr. Ulf Karlsson *KTH Royal Institute of Technology (Stockholm), Head of Delegation & coordinator*



Prof. Dr. Inger Andersson *Swedish University of Agricultural Sciences (Uppsala)*

Prof. Dr. Jens Birch *Linköpings University*

Prof. Dr. Annika Borgenstam *KTH Royal Institute of Technology (Stockholm)*

Prof. Dr. Aleksandar Matic *Chalmers University of Technology (Gothenburg)*

Prof. Dr. Gunter Schneider *Karolinska Institutet (Stockholm)*

Profiles of each member and personal contact details can be found on our website www.rontgen-angstrom.eu

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WHO CAN GET INVOLVED?

Any research group in Sweden or Germany currently working or planning to work on a project in the areas of Materials Science and Structural Biology and intending to use any of the involved large-scale research facilities is welcome to get in touch. A prerequisite is that the project is conducted together with a Swedish/German associate.

GENERAL CONTACT INFORMATION

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LARGE-SCALE FACILITIES FOR THE FUTURE: A SWEDISH-GERMAN VISION

Prof. Dr. Helmut Dosch, Coordinator of the RÅC and Chairman of the Board of Directors at the Deutsches Elektronen-Synchrotron (DESY)

With the establishment of the Röntgen-Ångström-Cluster in 2009, Germany and Sweden have embarked on a strategic initiative with a common vision: Future challenges of our society can only be mastered by joining forces in research, education and innovation. A core element in that strategy is the investment in modern research infrastructures and its effective utilisation in order to strengthen the scientific and technological capabilities.

Indeed, the large-scale research facilities which are now or very soon available in the two countries will give revolutionary new insights into the nanoworld. The Röntgen-Ångström-Cluster operates the most advanced suite of analytical tools world-wide for in-situ and in-operando studies of novel materials and for the molecular design of new drugs.

Since its beginning, the RÅC has made substantial efforts to contribute to this goal by supporting joint research projects and promoting young scientists. The framework of the Swedish-German collaboration allows an unprecedented level to fund, organise and conduct bilateral scientific activities with added values to both partners.

There are many opportunities that are ahead of this young Swedish-German cooperation. What has been primarily conceived as a bilateral cooperation can naturally reach out to other countries in the Baltic area. First steps have been made by including the Russian Federation into the trilateral RACIRI cooperation. The RÅC, on the shoulders of funding programmes of the German Ministry for Education and Research and of the Swedish Research Council, could serve as a nucleus and role model to advance the integration of further Baltic partners into a common research and innovation area.

Another opportunity is expected in strengthening knowledge gain and technology transfer from large-scale facilities to the industrial sphere. We know from many case studies that research infrastructures catalyse technological developments. In its future development, the Röntgen-Ångström-Cluster should draw from these experiences to further exploit the large innovation and technology potential at its facilities.

The Röntgen-Ångström-Cluster is now entering into the next phase with the start of the European XFEL in Hamburg as well as the MAX IV synchrotron and later the European Spallation Source ESS in Lund. This will further boost the international competitiveness of the Northern European Research Area and lift the power of the Röntgen-Ångström-Cluster for research and innovation to a new level. I am sure that this second phase will broaden the user base within the Cluster – in terms of geography but also with respect to scientific disciplines.

PROJEKTTRÄGER DESY (PT-DESY)

Projektträger DESY (PT-DESY) is a service provider for research management for its clients, mainly for the German Federal Ministry of Education and Research (BMBF). Established in 1974, the services cover the fields of project promotion, scientific communication and support for international research cooperation.

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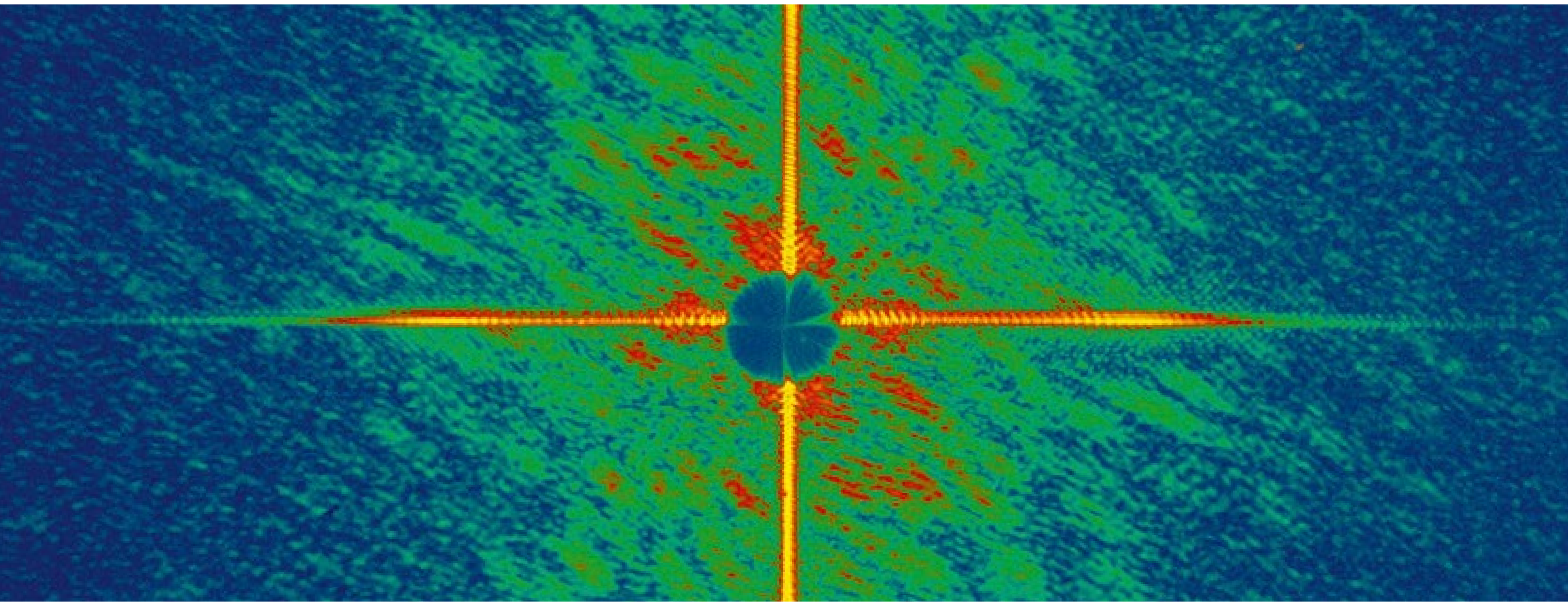

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