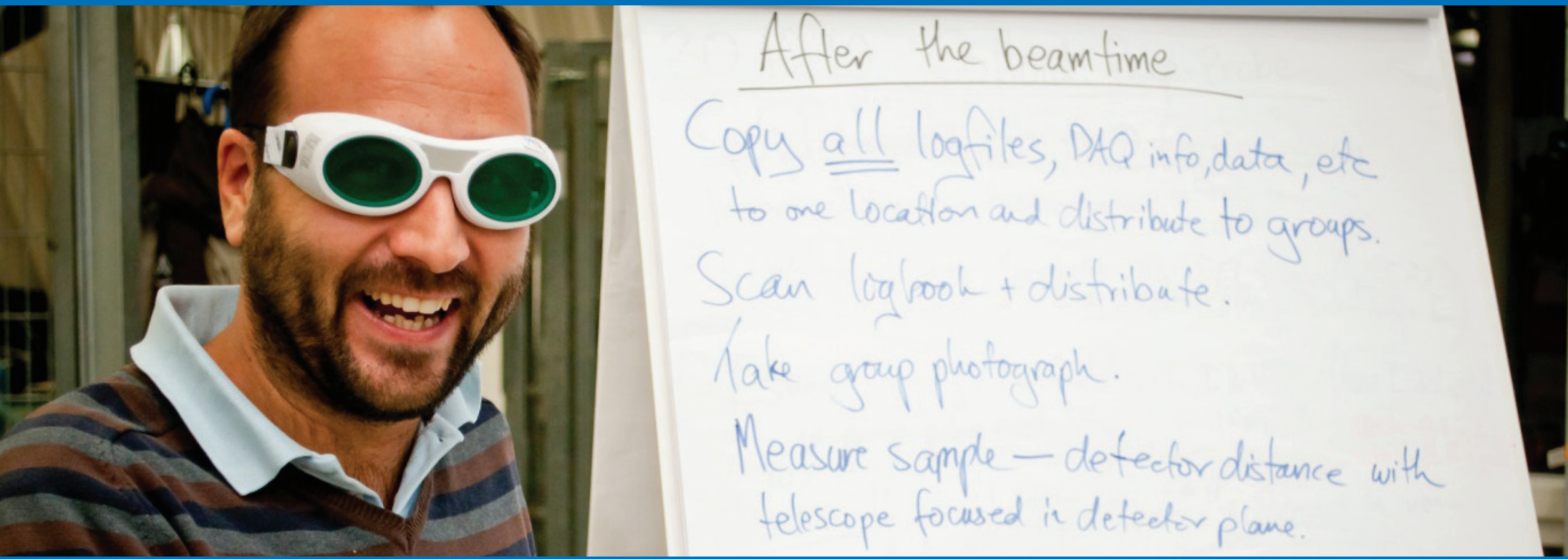
Röntgen Ångström Cluster



Instrument scientist Adrian Mancuso (photo: private)

PICTURE PERFECT – THE EUROPEAN XFEL IN THE MAKING

Can there be a more exciting place to work than the European XFEL? Adrian Mancuso doesn't think so. "When I was a student I would have never thought that something like the European XFEL would one day become reality", says the 34-year old Australian.

Adrian Mancuso is one of six leading instrument scientists working at the X-ray free-electron laser (E-XFEL) project in Hamburg. Mancuso's task is to deliver "the perfect instrument", more precisely, the Single Particles, Clusters and Biomolecules (SPB) instrument. In an ever progressing scientific environment his challenges are never ending. The Australian embraces them: "I like to be at the forefront of something I never expected could be realized. And I love to be creative and to find solutions."

Top scientists from around the world are involved in the ambitious project. "What we are doing is unique", says Adrian who has worked in leading research institutes in Japan, the US and Australia before joining the team in Hamburg. "Our laser will be the brightest in the world, and deliver 27, 000 pulses per second", explains Mancuso. At present, 120 pulses per second is the highest rate available worldwide.

With no comparable facility, Mancuso and his colleagues are starting every calculation from scratch. Mirrors required for the X-ray optics, for example, have never before been produced in the size and quality needed by the European XFEL. The scientists can spend days calculating, re-calculating and checking these calculations until they're confident their designs are just right.

The images that the European XFEL is expected to deliver via its revolutionizing techniques will help to understand the nature of biomolecules and other materials. This information can be crucial in the development of new drugs, for example.

"The demand for the European XFEL facility will be enormous", says Mancuso, adding laughingly "and by the time we're finished here, we should be looking at the next generation of scientific instruments. It never stops." Nonetheless, expectations are building up and scientists around the world watch impatiently as the work on site in Hamburg and its surrounds unfolds. Adrian Mancuso expects the assembly of his instrument to begin in 2015. From 2016 on, the facility will be open to researchers. (Background on page 4)

Editorial

German and Swedish scientists are busy working on their funded research projects to pursue the ever ambitious objectives of the Röntgen-Ångström-Cluster while others continue their efforts to bring the impatiently awaited new research facilities in Germany and Sweden on their way. Read about Adrian Mancuso's job at the European XFEL in Hamburg. His enthusiasm for the X-ray free-electron laser project is shared by many, not least the scientists waiting to use the revolutionizing facility which will be the only one of its kind in the world. The Helmholtz-Zentrum Geesthacht (HZG) is already adding significant value to the life of scientists and is committed to the aims of the Röntgen-Ångström-Cluster. Find below an interview with Wolfgang Kaysser, Scientific Director at the HZG. Last but not least, we introduce a few more funded projects in detail.

Enjoy reading! The editors

P.S. Make sure to visit www.rontgen-angstrom.eu regularly. It's an easy way to keep yourself informed about news, deadlines, forms, workshops, people, and projects!

Interview with Prof. Dr. Wolfgang Kaysser, Scientific Director of Helmholtz-Zentrum Geesthacht

Why is the Helmholtz-Zentrum Geesthacht involved with the Röntgen-Ångström-Cluster?

The HZG is located in Northern Germany and maintains good links with the Swedish scientific world as a matter of tradition. As one of the most important partners in the BMBF-supported ESS Design-Update project the HZG provides essential information in the fields of instrumentation methods, detector development and sample environment in order to prepare the construction of the ESS in Lund, Sweden. Additionally, the HZG runs the German Engineering Materials Science Center with several beamlines at PETRA III at DESY. For that reason, the HZG offers one of the most significant access points for materials research on large-scale facilities in Northern Germany and is thus a natural partner within the Röntgen-Ångström-Cluster framework.

Where would you place the importance of an international exchange between scientists nowadays and in the future?

Science has always crossed borders and competition takes place at an international level. In this context, the HZG sees itself as part of the world-wide sciences and nurtures an intensive dialogue and cooperation with organisations and individuals on all continents. The Röntgen-Ångström-Cluster ties in perfectly with these objectives because it facilitates collaborations with competent Swedish partners.

What are the opportunities that the Helmholtz-Zentrum Geesthacht provides for scientists?

Within the realm of the Röntgen-Ångström-Cluster the HZG enables scientists to access the materials-scientific beamlines at PETRA III at DESY referred to earlier.

The idea of the HZG is to establish longterm cooperations with external groups on top of the ordinary access via proposals. The objective here is to realize specific complex in-situ sample environments for joint research projects.

The Röntgen-Ångström-Cluster takes up this idea in an ideal way and supports suitable projects with Swedish partners.

Does the Helmholtz-Zentrum Geesthacht run events supporting the objectives of the Röntgen-Ångström-Cluster?

Since 2005, the HZG has been organising an autumn school dealing with materials research and neutron and synchrotron radiation every two years. This school will next take place in October 2013 as one of two R-Å-C-schools and intends to provide Swedish students with in-depth insight into these fields of research. (Photo: Helmholtz-Zentrum Geesthacht)

To find out more about the Autumn School in October 2013, visit www.rontgen-angstrom.eu (section announcements).

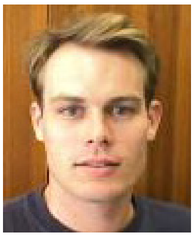
Employees at the Helmholtz-Zentrum Geesthacht © HZG

“Joint lubrication: structural reasons for high functionality” is one of the Röntgen-Angström-Cluster projects based at the Helmholtz-Zentrum Geesthacht.

„It runs like lubricate“. What is more often than not a standard phrase, is professor Regine Willumeit’s daily work. The Head of Department for “Structure Research on Macromolecules” at the Helmholtz-Zentrum Geesthacht analyses the “Joint lubrication: Structural reasons for high functionality” as one of the funded projects within the Röntgen-Ångström-Cluster. The aim of this research is to analyse the complicated interaction of joints, joint lubrication and cartilage. The project itself consists of two major parts where the first one aims at the development of two in situ sample environments. These will allow probing the structural arrangement of molecular assemblies under different shear and pressure conditions.

The second part focuses on the lubrication and load bearing properties of these components. Thus, combining the gained information will allow to draw a picture on the mechanisms which are responsible for the lubrication performance in joints and the findings will help to identify the properties which make the difference between good and bad lubrication. Therefore, not only procedures for the treatment of joint disease will be stimulated also friction minimization concepts e.g. in industry will be participate. (Photo: HZG)

Pilot project of efficient structural determination concentrating on the free-electron laser-carboxysomes
Project Coordinator: Dr. Anton Barty, DESY



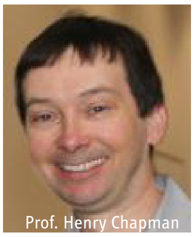
Photosynthetic marine microorganisms account for nearly half of the total carbon dioxide fixed into the biosphere while representing only about 1% of the total photosynthetic biomass on our planet. It has been hypothesized that the remarkable efficiency of this conversion process is due to the internal organisation and compartmentalisation of the enzymes responsible for photosynthetic carbon fixation. However, the internal structural organisation responsible remains unknown: intact carboxysomes are not suitable for 3D cryo-electron-microscopy and do not crystallize, thus cannot be imaged using X-ray crystallography.
We will use the newly developed technique of coherent X-ray imaging combined with newly available free-electron lasers (FLASH, E-XFEL) and conventional synchrotron facilities (PETRA III and the MAX facilities) to study the internal structure and function of the specialised organelles responsible for photosynthetic conversion in picoplankton. The unprecedented peak brightness of these sources enables X-ray diffraction measurements from single carboxysomes, which has never before been possible. (Photo: private)

A pulse-picking MHz Chopper for multi-dimensional angle-resolved time-of-flight spectroscopy at BESSY II (CHOPTOF)
Project Coordinator: Prof. Alexander Föhlisch, Head of the Institute for Methods and Instrumentation in Synchrotron Radiation Research, Helmholtz-Zentrum Berlin

Photoelectron Spectroscopy for Chemical Analysis (ESCA) has been a scientist´s window to the world of electronic structure and chemical bonding in matter of all aggregate states since the pioneering work of K. Siegbahn from Uppsala University (Nobel Prize 1981). One prominent achievement of Swedish-German collaboration in the past years has been the development of the angle-resolved time-of-flight electron spectrometer ArTOF in a collaboration of Uppsala University, the Swedish company VG Scienta, the Helmholtz-Zentrum Berlin (HZB) and the University of Potsdam. Compared to conventional hemispherical electron energy analyzers, an ArTOF has an up to 250-times higher transmission and can achieve an energy resolution, which is one order of magnitude better. The much higher detection efficiency reduces the acquisition time in experiments dramatically, allowing for dynamic, coincidence and high resolution experiments. The energy resolution of the ArTOF spectrometer is derived electron flight time – thus pulsed photon flashes are needed. Since at a synchrotron the bunch separation is typically too short, the goal of the CHOPTOF R-Å-C proposal is to integrate a mechanical MHz chopper picking X-ray pulses of the correct temporal distance. In this way a platform is created for the scientific use and further development of angle-resolved time of flight spectroscopy as a core of Swedish-German research infrastructure. (Photo: Helmholtz-Zentrum Berlin)

Combining and Optimizing Protein in vivo Crystallization and High-Throughput Serial Crystallography for Applications at the European XFEL and Third Generation Synchrotron Radiation Sources
Project Coordinator: Prof. Christian Betzel, University of Hamburg, Institute of Biochemistry and Molecular Biology; Laboratory for Structural Biology of Infection and Inflammation, c/o DESY | Prof. Henry N. Chapman, Center for Free-Electron Laser Science/DESY and University of Hamburg


Prof. Christian Betzel


Prof. Henry Chapman

The research project combines two topics aiming to optimize the future use of free electron laser (FEL) radiation and high-brightness synchrotron radiation in the field of structural biology. In terms of one sub-project the method of in vivo crystallization, established by the project coordinators and the collaboration partners Michael Duszenko (University Tübingen) and Lars Redecke (University Lübeck and University Hamburg), for the production of protein micro- and nano-crystals, to be applied for serial crystallography (SFX), will be analysed and optimized towards the design and construction of a semi-automatic platform for the production and scoring of in vivo grown crystals. The modular and transportable platform will be developed for automation and miniaturization of in vivo crystallization and will contain latest dynamic light scattering techniques to detect and score suspension containing micro- and nano-crystals. The possibility to produce and purify in vivo grown protein crystals automatically and on demand in close proximity to the SFX station will substantially increase the efficiency and flexibility of crystal sample production as well as delivery of appropriate crystal suspensions for SFX data collections and experiments. The research collaboration will apply and use for the in vivo crystallization functional proteins of Staphylococcus aureus bacteria and surface- as well as selected membrane-proteins of the parasite Trypanosoma brucei, a parasite causing sleeping sickness, as structural results will also support structure based drug discovery investigations.
A strong cooperation with Richard Neutze (University Gothenburg/Sweden) and Janos Hajdu (University Uppsala/Sweden) will allow the extension of in vivo crystallization for the production of membrane protein crystals, and will incorporate latest FEL based particle imaging methods. In terms of the overlapping second sub-project the method of serial crystallography (SFX) will be further developed, optimized and tested at the Petra III beamline P11 in close collaboration with the group of Alke Meents (DESY). In a first approach the highly focused beam will be used to collect diffraction data of protein microcrystals supplied in a flow-through mode in a capillary or a liquid microjet. Upon availability of the pink beam the expected high photon intensities will be utilized to obtain many thousands of single-crystal diffraction patterns from microcrystals, with microsecond exposure times. (continued next page)

Participants of the third German-Swedish workshop 'Opportunities and challenges of in situ methods for materials science with neutron and synchrotron radiation' in Hamburg © DESY

PEOPLE (CONTINUED FROM PAGE 3)

Latest detectors, such as the AGIPD, developed at DESY by Heinz Graafsma (project partner), will be used for this purpose, and software developed for FEL serial crystallography experiments will be adapted to merge the thousands of patterns. Furthermore, the sample delivery methods for FEL based SFX experiments will be optimized. A special light scattering system will be designed and adapted to the SFX set up, that allows a synchronization of sample delivery and detector response to optimize the yield of collected useful diffraction patterns relative to the number of crystals injected into the beam. (Photo: University of Hamburg)

EVENTS

Report on the third German-Swedish workshop within the Röntgen-Ångström-Cluster on topics in materials science

The workshop was the third in a series of German-Swedish meetings on topics in the field of materials science as part of the Röntgen-Ångström-Cluster. The workshop took place on the 18th and 19th of March 2013 at DESY, Hamburg, and was organized by Ulrich Lienert (DESY), Matthias Kreuzeder (DESY) and Astrid Holzheid (University of Kiel). More than 50 participants attended the meeting that has been supported by the Röntgen-Ångström-Cluster. The third German-Swedish workshop on materials science focused on in situ methods for materials science with neutron and synchrotron radiation.
Please read more on our website www.rontgen-angstrom.eu.

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BACKGROUND (CONTINUED FROM PAGE 1)

The Single Particles, Clusters and Biomolecules (SPB) instrument aims to image single particles by exploiting coherent diffraction imaging and associated methods using hard X-ray free-electron laser (FEL) radiation. Specifically, the SPB instrument will be designed to image single particles, which explicitly includes:
• Isolated, non-crystalline biomolecules
• Nanocrystals of biomolecules
• Atomic clusters
• Other isolated, single particles, in particular those of a "reproducible" nature

Furthermore, the SPB instrument aims to investigate the structure of these systems, as a function of time, through the use of so-called "pump-probe" measurements, where an optical laser excites a sample and the FEL probes it some delay time later.

The OTHER News

SWEDEN ON TOP WHEN IT COMES TO INNOVATION

New ranking shows EU more innovative, but gap between countries widening

The innovation performance in the EU has improved year after year in spite of the continuing economic crisis, but the innovation gap between member states is widening. This is the result of the recently published European Commission Innovation Union Scoreboard 2013, a ranking of EU member states.
While the most innovative countries have further improved their performance, others have shown a lack of progress. The overall ranking within the EU remains relatively stable, with Sweden at the top, followed by Germany, Denmark and Finland. Estonia, Lithuania and Latvia are the countries that have most improved since last year.