## THE FIRST SEVEN BEAMLINES AT MAX IV - and a more than thirty year long common history

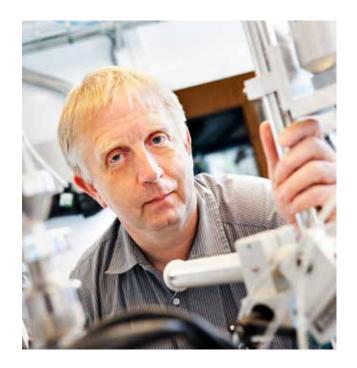


SEK 562 million is a lot of money! This is, however, the amount made available in the summer of 2011 for the construction of the first set of seven beamlines at the MAX IV Laboratory by the Knut and Alice Wallenberg Foundation (SEK 400 million) and twelve Swedish universities (SEK 162 million). The news that this generous funding had been granted marked the end of nine months of hard and exciting work on getting the application ready, discussing plans with Swedish universities, submitting the application and finally (and anxiously) waiting for the outcome of the KAW evaluation. In addition, this funding was on top of SEK 60 million previously granted by KAW for a postdoc programme for sending young researchers abroad to educate and prepare them for the future possibilities at MAX IV. With this funding in place the vision we all shared of building a set of beamlines exceeding all of the ones at the old MAX-lab and almost everywhere else in the world in terms of performance and science now became a reality! Needless to say, we are extremely grateful to KAW and the twelve Swedish universities for giving us this opportunity to make this vision a reality.

It is a great pleasure to thank the many people at MAX IV and at Swedish universities for their extremely dedicated work on developing the detailed plans for the beamlines in the application. Too many to be named here contributed to this work. Director Sine Larsen and Chair of the Board Lars Börjesson should be named and thanked for their work on securing funding, in particular but not only the funding from the Swedish universities. Travelling together with the two of you to Swedish universities for discussions with university management was a true and rewarding pleasure. Finally, Yngve Cerenius and Franz Hennies – who later established the Beamline Project Office (BPO) - must be thanked for their devoted contribution to the work of putting the application to KAW together.

Once the funding was secured, the hard work started on implementing the project structure outlined in the application, updating and securing time plans and budgets, preparing mandate and responsibility documents and reporting routines, discussing this with MAX IV Scientific Advisory Committee and the MAX IV Board, and generally getting everyone needed in the construction phase from MAX IV and Swedish universities on board. This also involved very enjoyable and fruitful discussions with Machine Director Mikael Eriksson on how to coordinate the beamline and machine projects. Again, it is a true pleasure to thank everyone involved for their dedication to the project and their very hard work.

Finally, the BPO and the beamline project managers and members at MAX IV and at Swedish universities, as well as the technical and financial staff at MAX IV are thanked for their work during the detailed design and construction



phase of the beamlines. You were certainly too few for what was to be accomplished, but in the true MAX-lab spirit you made up for that by performing way beyond what could reasonably be expected.

Thank you!

Hasle, 3 September 2018 Jesper Andersen Former Science Director of MAX IV Laboratory

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MAX-lab on Ole Römers väg was in operation between 1986-2015. Photo: Lars Davidsson (top) & Akademiska Hus (bottom)

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## **PREHISTORY 1986–2009**

## MAX-lab – KAW were involved from the beginning

The Knut and Alice Wallenberg Foundation (KAW) and MAX-lab have a long history together. MAXlab was opened to users with the MAX I ring in 1986 and KAW had already co-financed some of the instrumentation. The ensuing years entailed a build-up of MAX-lab where individual instruments were gradually added.

However, in the mid-1990s, it had become time for the largest investment to-date in connection with the construction of the MAX II ring, which also required an entirely new experimental hall. In this effort, KAW co-financed five beamlines with grants of SEK 46.5 million in total. The X-ray beam at MAX II could reach significantly higher energies than MAX I, broadening the user community, which also grew quickly with the expanded possibilities. This also came to be reflected in many applications to and grants from KAW for further expansion of the experimental possibilities at MAX-lab. During the years 1997 to 2009, nearly SEK 95 million was received for this in a total of 12 different grants from KAW.

MAX III, which was inaugurated in 2006, was in many ways a prototype for several of the design ideas that were subsequently fully implemented at MAX IV. MAX III also entailed a possibility to offer a synchrotron beam at lower energies as well, with significantly better properties than at the then somewhat aged MAX I ring. With the commissioning of MAX III and the beamlines on it, there were a total of 14 beamlines in operation on three storage rings. These beamlines were used by around 1,000 users annually. The user community was diversified and the experiments were about everything from seeking detailed information on the electronic structure of a material like graphene to solving the structure of a protein or studying what happens in a battery during a charging cycle.

Around 50 per cent of the users came from Sweden, in total two thirds from the Nordic region and the last third from the rest of the world. There was also a small, but important commercial activity, mainly at the high-energy beamlines at MAX II. Although the small MAX III ring was commissioned as late as 2006, it was clear to many people as early as the turn of the millennium that MAX-lab, mainly the large MAX II ring, could not be competitive for many years to come. Then, the large joint-European synchrotron radiation facility ESRF in Grenoble was in full operation at the same time that the new national facilities in England (Diamond) and France (Soleil) were about to start up. It would not take too synchrotron is an accelerator where charged particles (generally electrons) are accelerated to relativistic speeds and held in a circular orbit (storage ring) to produce synchrotron light. This takes place when the path for these particles is changed by a magnetic field.

The energy of the light produced depends partly on the electrons' own energy and partly on how much their path is bent. The energy and thereby the wavelength for the synchrotron light can vary over a wide range. Wavelengths from infrared light via visible light up to soft and hard X-rays can typically be covered. Compared with the light from a conventional X-ray source, synchrotron radiation also has a number of other interesting properties.

The largest difference is the several orders of magnitude higher intensity (or rather brilliance, a unit where consideration is also taken to source size, divergence and bandwidth). The synchrotron light is also significantly more collimated; it can be coherent, especially on MAX IV, and polarised. All of this together makes the synchrotron light particularly attractive for many applications and experiments that are done on beamlines around the storage ring.



many years before MAX-lab would be left in the dust by technical development.

An intensive endeavour began to study possibilities and designs for a new synchrotron facility in Lund. KAW was involved and financed also this by granting an application for SEK 14 million in 2002 for the "Development of the next synchrotron light source in Sweden".

As it is not within the scope of this text to go into the details of the intense and innovative design development on the accelerator side that took place under the leadership of Mikael Eriksson, Professor of Accelerator Physics and also the Machine Director at MAX-lab, the interested reader is referred to other sources, such as: The Marvelous Light in Lund – How MAX IV Came About (2016) ISBN 978-91-7623-868-4

Here, we briefly note that at the beginning of the 2000s, development was in full swing to design a completely new synchrotron radiation facility that could offer entirely new and world leading performance, as well as possibilities for the beamlines that would be built at it. The explicit goal was for MAX IV to entail a generation change in terms of the design and performance of a synchrotron.

#### Establishing support and priorities How to choose seven beamlines?

It was hardly realistic to expect that the first MAX IV financing, if and when it would ever come, could also cover all of the beamlines and experimental techniques one may have wanted to offer the users at MAX IV. Directly replacing the 14 beamlines that were in operation at MAX-lab with 14 entirely new beamlines was not up for discussion or even technically possible. Priorities had to be made. There were many aspects to take into account in such a prioritisation process. Strong national and international user communities and scientific expertise in various experimental methods and their use had been built up around the beamlines that were in operation at MAX-lab. At the same time, the predicted characteristics of MAX IV entailed entirely new possibilities. Now, synchrotron light could be created with absolutely world leading characteristics with regard to brilliance and coherence from the soft to the hard X-ray regime. This paved the way for entirely new techniques that could use these characteristics. Here, it was important to find a suitable balance between these and other considerations.

The foremost examples of strong and well-established user communities at MAX-lab were among the various soft X-ray spectroscopy methods, such as XPS (ESCA) and Arpes. Many of these users had been involved in building up the activities from their inception in the mid-1980s. With their expertise, they had made incredible contributions to MAX-lab's development and strong international position in soft X-ray spectroscopy methods. Entirely different techniques could also be said to be well-established at MAX-lab. In connection with the possibility of achieving higher energies at MAX II, mainly with the help of the superconducting insertion devices, environments were built up very fast around various X-ray scattering methods and EXAFS at the beamlines I711, I811 and I911. Naturally, we wanted to also offer these users a continuation at MAX IV.

Especially since the higher energy at the MAX IV ring would offer these users significantly better possibilities than at the old MAX II ring.

## MAX IV CDR – An initial design and an initial list of beamlines

The process of identifying suitable beamline proposals essentially began at the same time as the initial discussions about a new accelerator in Lund. To mention some important highlights in this process, a starting shot was the three-day conference in Lund "Our future light source", which was held in 2004 and from which several different working groups crystallised around various techniques and areas of science. In 2006, the work was able to be documented in the 333 page book "MAX IV CDR – Conceptual Design Report". In it, both the new accelerators and 24 beam-

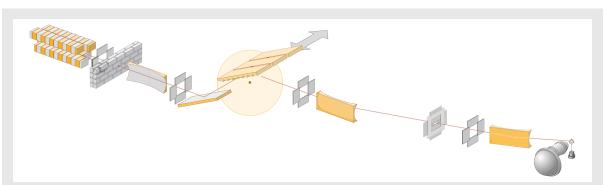


lines were described at a conceptual level. These beamlines were intended to both use the new possibilities of MAX IV, but to also meet the conceivable needs mainly in the Swedish user community. In connection with this, a few but very important and strategic decisions were made.

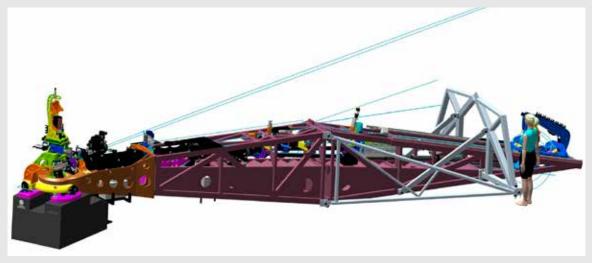
One was to not exclude a future development towards a so-called Free Electron Laser (FEL), but that the majority of the intended user community above all sought experimental techniques based on synchrotron light. Another was that MAX IV would entail an investment in both soft and hard X-ray techniques.

The new facility thereby not only needed to cover a broad wavelength/energy range from a few eV up to a few tens of keV, but also needed to offer optimal performance over this entire interval. This was to some extent different from most other facilities, which most often prioritised a certain energy range and indicated that MAX IV would need to consist of more than one storage ring. All seven of those that ultimately became the first phase beamlines can be traced back to proposals in this CDR.

The process continued in the subsequent years with, among other things, a series of very well-attended user meetings at MAX-lab, around 300 participants per meeting, during the period 2005-2009. These meetings had seminars that were focused on various techniques and possibilities of MAX IV. They entailed an opportunity to further refine the earlier proposals and some beamlines crystallised as natural choices to be included in a first wave.



A schematic illustration of a typical spectroscopy beamline at MAX IV. Furthest left is the insertion device, placed on the inside of the ring tunnel, followed by the part of the beamline called the front-end where water-cooled apertures and shutters provide an initial definition of the beam. Outside the ring tunnel is an initial mirror to focus the beam followed by a monochromator where a certain wavelength (energy) is chosen followed by mirrors and apertures used to focus the beam before it hits the sample. In this case, the electrons sent out from the sample are analysed in an electron analyser furthest right. Illustration: Johnny Kvistholm



The extremely advanced spectrometer arm at Veritas is one of many results of successful collaborations between MAX IV and the various Swedish universities. The set-up was designed and built at Uppsala University and is now being put into operation on the beamline. Illustration: Carl-Johan Englund

beamline is the common name for an experimental station at a synchrotron. However, the beamline consists of significantly more parts than the actual experimental set-up that the users encounter when they come to a facility like MAX IV.

It begins in the storage ring where the electron beam produces synchrotron light. On MAX IV, this is only done at insertion devices, which are extra strong magnet structures that are placed on the roughly 5-metre long straight sections that are between every seven bending magnets around the ring. The light produced in these insertion devices is then initially defined in the part of the beamline called the front-end.

These first two parts of the beamline are placed inside the thick concrete walls of the actual storage ring. Outside the ring is first the optics where the synchrotron beam is further defined, generally by being focused and monochromatised. There are various kinds of optics to focus an X-ray beam.

Most beamlines at MAX IV use very weakly curved super polished mirrors where there is nearly 100 per cent reflectance at small incident angles and where the curvature means that the beam can be focused on e.g. samples or detectors.

As a rule, a certain wavelength (energy) is chosen for an experiment. For beamlines designed for lower energies, this is done with various kinds of artificial gratings while for beamlines with higher energies, this is done with crystals, e.g. Si (111). The actual experimental station comes last and is the part of the beamline that the users come into contact with and the samples are mounted here and there is some form of detector for the reading of data.



Signing of the financing decision for MAX IV. From left Pär Omling, Director-General Swedish Research Council, Per Eriksson (standing), Vice-Chancellor Lund University, Jerker Swanstein, Chairman Region Skåne, and Mats Helmfrid, Chairman of the Municipal Board in Lund. 05

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## FINANCING AND APPLICATIONS 2009–2011

#### Financing decision in 2009

On 27 April 2009 at Biskopshuset in Lund, an agreement was signed between the Swedish Research Council, Lund University, Region Skåne and Vinnova, which came to secure the financing of what at the time was called an initial version of MAX IV. There are probably few who believe that it was a coincidence that this decision was made just days before the allocation decision of the European Spallation Source (ESS) to Lund. At the same time, it was the result of a long and successful effort with many people involved, especially MAXlab's management with Director Nils Mårtensson and Machine Director Mikael Eriksson leading the way. The financing for this initial version of MAX IV came to cover the accelerators and some peripheral facilities, e.g. chemistry labs and workshops. At the same time, the discussions continued on how a first wave of beamlines would be financed and which beamlines would be included. A number of stakeholders were naturally involved in this process: the Swedish universities, representatives from industry, MAX-lab's own experts, the user association, advising committees and the MAX IV Board. Claiming that the process was simple and that the choices were given would be an exaggeration and in the financing decision for the actual facility, the situation was still somewhat unclear.

The process continued in 2009 and in Febru-

ary 2010, a well-visited and important three-day workshop "Beamlines at MAX IV" was held where 24 beamline proposals were presented in total.

After this, the recommendations from MAXlab's Program Advisory Committee (PAC) and the reference group from the Swedish universities, there was finally a list confirmed by the Board of a total of ten new prioritised beamlines and a number of beamlines that should be moved from the old MAX-lab to MAX IV.

The ten prioritised (new) beamlines were divided into three categories according to:

#### Highest priority

- Very High Resolution Soft X-ray Spectroscopy (Veritas, I)
- High Pressure and High resolution Electron Spectroscopy (HIPPIE, I)
- A Short-Pulse Facility for Time Resolved X-ray Science (FemtoMAX, I)
- Nanofocus Beamline (NanoMAX, I)
- Life Science Beamline Microfocus (Micro-MAX, III)

(Just) Slightly less priority:

- Angle Resolved Photoelectron Spectroscopy (Bloch, I)
- Gas Phase Core-level Spectroscopy (partly taken over by FlexPES, II)

Extremely important to secure continuity:

- A SAXS/WAXS beamline (CoSAXS, II)
- Hard X-ray Environmental XAS Spectroscopy Beamline (Balder, I)
- Life Science Beamline: High-throughput and phasing (BioMAX, I)

All of these beamlines have entirely or partially become a reality, or in any case, commenced projects at MAX IV. Shown in parentheses are the names that the beamlines now have at MAX IV and the phase in which the financing for the beamline was ultimately secured (I, II or III).

In this context, it is worth mentioning that one beamline at MAX IV is in itself a very large project with a typical budget of up to SEK 100 million. In order to be able to meet the high expectations, entirely new requirements were set on both instrumentation and associated infrastructure. These beamlines were something completely different than the ones at the old MAX-lab where underfunded projects were often begun and the build-up of a beamline could draw out over a long time with various financiers and with home-made budget solutions. The high expectations at MAX IV meant that the requirements were significantly tougher both in terms of the actual hardware, but also the construction process. It was absolutely clear that the accelerators

would come to provide opportunities to produce an X-ray beam with absolutely unique properties and it was never an option to build beamlines that could not fully utilise their performance. This also unavoidably affected the budget for the beamlines.

#### The first KAW application in 2010

It was probably with somewhat great expectations that the first application to KAW was submitted in spring 2010, formally by the Swedish Research Council (VR) and not by MAX-lab. This application concerned financing of six beamlines (of the previously mentioned prioritised ten) for a total of SEK 500 million and SEK 60 million for a scholarship programme for young Swedish researchers to enable their research at facilities similar to MAX IV. Rather soon there were indications that the scholarship programme would be granted as an important support for a new generation of Swedish synchrotron users. The beamline part of the application was not approved, however. MAX-lab was instead welcome to return with an application for a maximum SEK 400 million no later than 1 April 2011 (later extended by one month). This new application should have better documentation on how to ensure that these beamline projects could be realised and how support for them had been established.

KAW also asked MAX-lab to especially address nine issues, which KAW did not consider to be fully established in the first application. Examples of such issues were:

- The Foundation expects an account of the prioritisation process that formed the basis of a revised application. Here, the Foundation wants to specifically point out that the Foundation's country usefulness responsibility must be taken into account in the prioritisation.
- The Foundation wants an account of the organisation and responsibility for every prioritised beamline.
- The Foundation expects a revised application based on detailed design reports for proposed beamlines, including independent international evaluation of the respective design concept.
- The Foundation expects an account of the intended structure of collaboration between the MAX IV laboratory and Swedish research teams that can be considered central to the design and use of a specific beamline.

#### The second KAW application in 2011 – redo, do right

MAX-lab therefore had to redo and do it right. There were numerous issues that were thereby addressed at an entirely different level in the second application. In this context, MAX-lab also changed its name to MAX IV, which accordingly became the collective name for both the activities at the old MAX-lab and the MAX IV project. Leading the work on the new application and the associated organisational issues landed on the desk of the new Science Director at MAX-lab/ MAX IV Jesper Andersen. As a professor at the Division of Synchrotron Radiation Physics at the

Department of Physics of Lund University, he had been involved in building up MAX-lab and used its beamlines for many years and naturally had very good knowledge of both the operations and the challenges that the laboratory now faced. The work on the application was also facilitated by KAW's somewhat detailed questions. However, the Foundation also wanted "a proposal on the financing of prioritised beamlines based on the Alice and Knut Wallenberg Foundation contributing a maximum of 75 per cent of the total cost of an individual beamline". In other words, besides seeking answers to a number of specific questions, KAW also sought co-financing of 25 per cent. If this could be secured, KAW could grant framework funding of up to SEK 400 million. A natural partner in this issue was the Swedish universities, which had used around 50 per cent of the available beam time at the old lab and over the years had both invested in and built up, and in some cases also operated, a number of beamlines.

MAX IV was naturally in continuous contact with these universities and there was a preparedness to discuss a possible co-financing out at the universities. After a Board decision, the time was used to continue the work on all ten prioritised beamlines.

## Collaboration with Swedish universities and research teams

Already from the beginning, virtually all of the 24 presented beamlines in the MAX IV CDR from 2006 were well supported at the Swedish

universities in so far as there were enthusiasts who propagated for and had experience of these very experimental techniques. The author list of around 300 names spread over around 100 different institutions already indicated this. This support, however, needed to be strengthened and formalised and KAW pointed out the "beneficial to Sweden" perspective in particular. A system of spokespersons and advisory groups that were found spread over Swedish universities were tied to all ten prioritised beamline projects, and the working groups that continued the design work also generally included representatives from various Swedish universities. It was naturally important as the discussion on co-financing from the universities continued in parallel, but also because for several beamlines the expertise was stationed at a university rather than at MAX IV. In the work of preparing detailed descriptions of the ten beamline projects, MAX IV extensively used these groupings as writing groups for the second application. These groups and persons generally continued to be very important for the beamlines throughout the entire project period.

#### Design

The beamlines could now be described up to a relatively detailed level and, just before the second application was sent into KAW, an evaluation was also conducted of the respective beamline by external experts as a part of the final prioritisation process, also described in the below section on "The application and the final prioritisation".

In addition, a process was described where a

further external examination was also to be done of the detailed beamline design before any procurements were initiated. What came to be called DDR (Detailed Design Report) became the most important control point in the beamline projects and there is reason to come back to these.

#### Budget

The work of preparing a more detailed budget continued during the year. In itself, this was a somewhat large challenge as every beamline consists of thousands of parts where many components are so unique that they must be developed solely for this beamline. What was also new was that the infrastructure became so much more expensive than for beamlines at the old MAXlab. The requirements were completely new and earlier experiences often proved to be irrelevant. These kinds of costs are often difficult to identify and compare between various synchrotrons as they can be hidden in other items, such as salaries for a larger support organisation.

Fully using the performance that can be offered at MAX IV at the same time means that extensive resources must be invested in infrastructure. To mention one example, focusing an X-ray beam down to a size of a few nanometres not only places major demands on the source and optics, but also on issues like temperature stability.

A modern research facility also sets entirely new requirements concerning to both personal and machine safety.

One way to reduce uncertainty with regard to the total budget despite the uncertainty in the

## Some typical numbers on infrastructure for a beamline at MAX IV

Network cable	2000 metres
Motor cable	1000 metres
Water cooling pipe	200 metres
No. of engines	100 pieces
Lead for radiation shielding	40 tonnes
No. of cooling water systems	6 pieces

individual figures was to use so-called three-point estimates. The principle is somewhat simple: an estimate is done of a pessimistic value, an optimistic value and a value for the normal and seeks to weight these. This approach was successfully used primarily on large and unique items, such as insertion devices, optics and detectors where a single item could be budgeted at several million SEK. The total budget limit was known (a maximum of SEK 562 million) so the question was how many of the prioritised beamlines could fit within this limit. In this process, some options for several beamlines were removed, such as a second side station or several different detectors.

#### **Project organisation**

MAX IV would show that they could build up a project organisation that did not exist before. This needed to address project coordination on several levels. The beamline projects must be coordinated with each other, as well as with the build-up



Happy and hopeful project managers and representatives of the BPO in a row in front of the large experimental hall during the MAX IV building project in August 2013. Photo: Franz Hennies

of the accelerators and experimental halls. These three main projects were to take place virtually in parallel where the build-up of the accelerators would require the absolute majority of MAX IV's own internal resources. At the same time, operations at MAX-lab were still under way and personnel were naturally required to make sure they continued. In order to address these challenges, a number of reinforcements and clarifications in the line organisation took place and an entirely new project organisation was built up at MAX IV. The project organisation that was put into place and which remained active until the accelerators were commissioned was described for the first time in the second KAW application. Central to the organisation was a project coordination group with representatives of the accelerators, beamlines and the construction project, as well as support functions such as finance, IT and workshops. This group was led for several years by Allan Lidforsen, an external consultant who reinforced MAX IV with project management expertise during this hectic period. The project coordination group was to balance the needs of the operation of the old facility, the beamlines in the project phase at MAX IV and the accelerator projects and lastly the construction project, which indeed located at an external company (PEAB), but needed extensive coordination with the other projects.

At the next level, the various beamline projects needed to be coordinated with each other. Both in terms of resources and time, but also to find common technical solutions and project tools that could work in the MAX IV organisation, for example. This was done through the formation of a project office, the Beamline Project Office (BPO), which worked with the project managers for each of the beamline projects and was led by the Science Director.

#### Project managers (PM)

The most important role in the beamline projects and where it was most pressing to appoint a person was the project manager. The project manager role as it was chiselled out had an extensive breadth; it meant that the person had a scientific and technical, as well as a financial responsibility for the respective beamline. The beamline was not only to deliver the experimental possibilities described in the application, but also fulfil a number of requirements with regard to technical and safety standards, while at the same time follow procedures for reporting, the Public Procurement Act, etc. All of this was to be delivered in an organisation that previously had little experience in many



Sun shining on BPO! Here Andreas Lassesson, Yngve Cerenius and Franz Hennies going through installation plans.

of these areas. The project manager was also the contact point for the respective beamline project, which did not necessarily have to be (completely) located at MAX IV, but rather could have its centre of gravity at a Swedish university, for example.

It was natural that those who helped write the respective section of the application and prepare a preliminary design of the beamline also continued as project managers. This was simplified by the fact that in most cases it was possible to see the first MAX IV beamlines as a logical continuation of an existing activity at MAX-lab. There were thereby people with both scientific and technical anchoring in the respective technology.

Beamlines at MAX-lab	Beamlines at MAX IV
1911	BioMAX
D611	FemtoMAX
1811	Balder
1511	Veritas & HIPPIE (also SPECIES)
13 & 14	Bloch (Arpes)

The new MAX IV beamlines naturally entailed completely new performance and thereby new possibilities compared with the corresponding beamline at MAX-lab, but it was actually only NanoMAX that could be said to be the beginning of an entirely new activity and there was consequently little experience at the old lab to fall back on when the project was to begin. However, it was a given choice that MAX IV would have a "nano beamline" from the beginning to fully utilise the new performance that the 3 GeV ring at MAX IV offered.

#### Spokespersons

A spokesperson for a beamline has to fulfil two challenging criteria. Firstly, they must understand the intricacies of MAX IV and the difficulties associated with building beamlines from the ground up. Secondly, they must be acutely aware of the needs and desires of the user community of the beamline. Finding both criteria in a single spokesperson is rare but essential to the MAX IV project which aims to build a world leading user facility. Without user input, MAX IV cannot serve the community and without feedback from the beamline staff, the equipment will never work. As it happens, many of the spokespersons have been users of MAX-lab for many years and consider themselves users of the new facility. In this way, they have had time to understand the inner workings of a synchrotron and yet still fit firmly within the user community themselves.

That is not to say that contact with the users should be taken for granted. The spokespeople worked tirelessly to continually engage with the users although the requirements in each field were different.

Ingmar Persson, the spokesperson for Balder recounted how he organised many courses over the years starting in 2005 called "XAFS for beginners". The courses were very popular and often attracted more than 30 people at a time and more than 400 people have taken the course overall. The purpose of the course was to educate new users about the techniques and eventually to create discussions and anticipation of the Balder beamline as it was under construction. By running an introductory course, Ingmar Persson hoped to attract users who had never considered using XAFS before from fields as diverse as biology and archaeology. The hard work eventually paid off when Balder was funded owing to the strength and support of the user community.

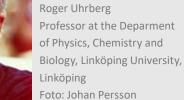
Roger Uhrberg, spokesperson for Bloch also took the user interaction very seriously. Every time he approached discussions around the beamline, he did so from the point of a user. He was particularly concerned with delivering the highest quality instrument to the user community, balancing the need to produce high quality with a sense of urgency, "too early and it's not good enough, but we also have to minimise the downtime for users" said Roger Uhrberg.

Gunter Schneider, the spokesperson for Bio-MAX, made intelligent use of the well organised structural biology research community in Sweden. They host regular meetings so it was easy to keep them informed of developments and ask for input when needed. Coupled with specific work-



Ingmar Persson Professor at the Department of Molecular Sciences, Swedish Agricultural University, Uppsala Foto: Viktor Wrange

Gunter Schneider Professor at the Department of Medical Biochemistry and Biopysics, Karolinska Institutet, Stockholm Foto: Ylva Lindqvist



shops the contact with the researchers has always been strong. "It felt like everyone was heard and there was very little disagreement", said Gunter Schneider, reminiscing that perhaps one of the only frustrations was that the structural biology community was only getting one beamline and not two (in the first phase).

Another vitally important role of the spokesperson was to help to secure funding. Each beamline working group had to make the strongest possible scientific case in order to be granted the money to build the beamline. During this process the beamline staff worked hard with the spokespeople. In this process, good communication was essential. Roger Uhrberg spoke about how he was always on the phone to project manager Balasubramanian (Balu) Thiagarajan. Other spokespersons had different approaches to communicate with the beamline team, but all of them took it very seriously as well as taking the responsibility of making the scientific case and securing funding personally. For many of the spokespeople, this was a great deal of fun. As a synchrotron user, you almost never get the opportunity to design your own beamline. Roger Uhrberg described the feeling that in the meetings to discuss the design, it felt possible to bring up all of your frustrations about present day instruments and fix them. If you need special photon energies, sample environments or detectors, now was the time to make changes. "During the design process, our frustrations became opportunities," said Roger Uhrberg. There are always difficulties within complex projects like this, but it was very hard for the spokespersons to recount them. Gunter Schneider says "you have to understand, I'm not just a user of synchrotrons, I'm a fanatic". While not everyone spoke so emphatically, the passion for the project across the spokespersons was clear. They were very engaged and excited by the projects and problems did not register as problems to them. Instead, they seemed more like interesting challenges that had to be discussed and overcome. This is both a testament to the focus of the spokespeople, as well as the hard work and competence of the beamline staff who worked tirelessly to execute on discussions and ideas. There are of course always frustrations with projects and the biggest has been delays in the beamline construction. While the spokespersons felt the frustration, they were largely philosophical about them, remarking that on the whole, the projects had been incredibly well executed. Delays are unfortunate and disappointing to everyone involved, but they are not uncommon and they will be overcome with the same enthusiasm and hard work that has got the project this far. All of the spokespersons were very quick to cite important members of the team that had made the project a success and who would steer the project past the delays to completion. As Gunter Schneider put it, "it's the people who make the project".

Given the passion and enjoyment that each spokesperson expressed for their projects you would imagine that there would be something that they would miss from the project phase. The surprising answer was an almost categorical, no. The simple reason for this is that upon completion of the beamline, each of the spokespersons now sees themselves as users of the instrument they have helped to create. This is probably like asking someone who just sat down in front of a huge cake if they missed anything from the baking phase. Every spokesperson was very eager, almost impatient to try out their brand-new instrument. It represents the fruition of over a decade of work for some of the spokespersons, so it is understandable that this close to the finish line, they are excited to try it out.

#### The application and the final prioritisation.

All ten prioritised beamlines could not fit in the given budget limits so a final prioritisation needed to be made. The first step was that all proposals were evaluated by international experts who looked at technical and scientific aspects, such as how well these beamlines utilised the performance of the accelerators, feasibility and design. They also evaluated the projects' budgets and timetables. This evaluation together with input from the research teams that contributed to the process and the MAX IV Science Advisory Committee (SAC), a list of seven prioritised beamlines was prepared by the management of MAX IV and was confirmed by a Board decision. To be able to fit into the predefined budget limits, some projects also had to be trimmed down a bit. This was done by certain options being removed, such as a second experimental station being put on ice while what was left in the projects was fully financed up to the necessary level.

Beamline	Project leader	Spokespersons
Bloch (Arpes)	Balasubramanian Thiagarajan	Roger Uhrberg, Linköping University
Balder	Katarina Norén	Ingmar Persson, SLU Uppsala
BioMAX	Thomas Ursby	Gunter Schneider, KI and Richard Neutze, University of Gothenburg
FemtoMAX	Jörgen Larsson, Lund University	Jörgen Larsson, Lund University
Hippie	Jan Knudsen	Joachim Schnadt, Lund University
NanoMAX	Ulf Johansson	Anders Mikkelsen, Lund University and Ulrich Vogt, KTH
Veritas	Marcus Agåker, Uppsala University	Jan-Erik Rubensson, Uppsala University
	that came to be included in the application is not given, it is MAX IV.	ation to KAW 2011 with project leaders and spokespersons.

The 747 page thick application "An initial MAX IV beamline program" (unofficially called the Jumbo Jet) for a total SEK 400 million was finally sent in after feverish work a few minutes to midnight on 30 April 2011.

The work was led by Jesper Andersen who was the Science Director at the time and was largely structured according to the project model that had already been described with somewhat independent writing groups that were often located at the universities, but had a local contact person at MAX IV, and where the coordination was then done by Jesper Andersen and the BPO. It came to especially address the questions that KAW had asked in response to the earlier application. It was also able to present a financing model where the 11 largest Swedish universities, from north to south: Luleå University of Technology, Umeå University, Uppsala University, the Swedish University of Agricultural Sciences (SLU), Stockholm University, the KTH Royal Institute of Technology (KTH), Karolinska Institutet (KI), Linköping University, the University of Gothenburg, Chalmers University of Technology and Lund University, would supplement the KAW grant by a total of SEK 160 million. In this process, Karlstad University also added another SEK 2 million dedicated to the Bloch beamline.

The answer came on 4 July 2011 and KAW promised framework funding of SEK 400 million for the construction of these seven beamlines!

The winning architect proposal from FOJAB Architects. The final design was slightly different (see cover photo). 1.31

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## PROJECT PHASE 2011–2017

At the end of 2011, the funding was set for the first seven beamlines, a project organisation for them was described and the construction of MAX IV had begun. As previously mentioned, the MAX IV project was divided into four main projects: The Construction, the Accelerators, the Beamlines and the Operation of the old lab. A brief introduction to the other projects may be appropriate before delving deeper into the beamline projects as all of them interact with each other to a very large extent.

#### The Construction project

It was clear that the core activities (both beamlines and accelerators) would place very large and, for the construction companies, somewhat special demands on the property. This concerned everything from design, infrastructure to the need for stability. The latter concerned both the sensitivity to external and internal sources of vibration, as well as temperature stability on the premises or in various cooling water circuits. Stability requirements on the floor down to some 20 nanometres were discussed at the same time that a temperature stability of ±0.1° was required for certain critical cooling water systems and in some especially sensitive premises, such as around the experimental set-up at NanoMAX. MAX IV needed to define the requirements so that a procurement process could be done and then together with the winning company, which turned out to be PEAB, add further details regarding these issues. A 25-year lease was signed at the beginning of 2010 with Fastighets AB ML4, a jointly owned company established by PEAB and Wihlborgs especially for this purpose.

The exterior design of the building was done by FOJAB after an architecture competition arranged by the Municipality of Lund. It met both high aesthetic standards, but was also flexible in the

## Some examples of stability requirements defined during the building process:

Temperature stability experiment hall	: ±1°
Temperature stability	
NanoMAX experiment hutch:	±0.1°
Delivered maximum heat output in the hall per beamline:	1.5 kW
Temperature stability critical water cooling systems:	±0.1°
Avoid natural frequencies below:	55 Hz
Target value for acceptable amplitudes of floor vibration:	20–30 nm (vertically)

sense that it should be relatively easy to expand with new premises for beamlines or laboratories. PEAB set up a project organisation that enabled extensive participation from MAX IV that was to use the premises. The activities' requirements and especially the requirements from the beamlines were largely able to define the building. The exterior physical design, the doughnut shape, enabled up to 50-metre long beamlines without having to go outside the building's exterior wall. For some beamlines, this was not enough. An optimal design for NanoMAX required it to be at least 100-metres long. MAX IV was therefore project engineered from the beginning with an extending satellite building for this beamline. The design of Veritas also required special adaptation of the premises. Here, a 54-metre long beamline was needed where an 11-metre long arm at the furthermost point could rotate up to 120 degrees around this point. This was also made possible by optimising the placement of the beamline and an extra "lemon slice" within the building.

#### Adapting the premises to the activities

Innumerable drawing reviews were done to ensure that the premises met the requirements from MAX IV. Details such as the placement of the lead-throughs on the accelerator tunnel, the

Photo taken inside the tunnel of the3 GeV ring with a yellow seven-bend achromat and the blue undulators for HIPPIE and Veritas in the background.

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need for cooling power in various electronics racks or temperature stability as a function of the height of the experiment hall were nailed down in great detail. MAX IV received the necessary structural engineering expertise through a few key recruitments, Caj Lundquist and Jacob Schuster, that joined the project early on. PEAB set up a process at the same time to ensure that MAX IV's requirements could come in as late as possible in the building process, but still in a structured manner. This way, the construction project could continue quickly and smoothly at the same time that MAX IV had their wishes heard.

PEAB also demonstrated great flexibility by permitting access to MAX IV to begin their own installations while the construction project was still under way. The results can be said to have been very good in the sense that construction both went faster and at a lower cost than was first estimated at the same time that the wishes from MAX IV were captured in an excellent way. Perhaps not everything was discovered this way, but there were no major issues even if many might have been a bit surprised to one day find an evacuation route from the underground klystron tunnel that runs parallel to the linac, in the middle of the floor of the 3 GeV ring's experiment hall.

On 1 June 2015, ML4 formally turned over the key to the MAX IV facility to Lund University. That same year, MAX IV was named the best project both in Green Building and BREEAM at the Sweden Green Building Conference. As early as 2014, MAX IV was named the Best Futura Project at MIPIM in Cannes.

#### The Accelerator project

The Accelerator project can naturally be divided up into three parts: the roughly 300-metre long linear accelerator (the linac), the large storage ring with a circumference of 528 metres and the small storage ring, 96 metres in circumference. Purely chronologically, the linac would be finished first. The two underground tunnels for the linac and the associated electronics (the klystron gallery) were the first parts of the MAX IV building that were ready for occupancy so that the installations could begin in January 2013. These then continued during the year and the first tests were carried out in summer 2014 when permission to begin operations was obtained from the Swedish Radiation Safety Authority (SSM). In direct extension of the linac, there is an experimental operation called the Short Pulse Facility (SPF) with one of the first phase's KAW beamlines, FemtoMAX. The original idea was that the linac and Femto-MAX would be finished significantly earlier than other parts of the MAX IV operations and could thereby take in users early in the project. Unfortunately, it turned out during the project period that this could not be prioritised and the first experiments were done at FemtoMAX at roughly the same time as the other KAW beamlines.

#### The 3 GeV ring

The large storage ring was up next and for this, a prototype had been built of an achromat (section) next to the old MAX-lab. This was to be able to practice the various steps that would take place during the installation and see how the various infrastructure sections could be installed optimally around the magnets. The installations began in June 2014. The large ring consists of 20 achromats with seven unit cells each. Each of the 140 cells is around three metres long and has innumerable functions that are each to be cabled and functionally tested.

The MAX IV design is unique precisely with regard to these unit cells with several different magnetic functions incorporated in the same iron block. This set extensive requirements as to tolerances in production, but at the same time made it possible to achieve hard alignment tolerances with a reasonable effort at installation. This naturally not only involved MAX IV's own personnel, but also many external electricians and plumbers. Another somewhat odd element of the flora of external resources that helped out during this period was the accelerator specialists from the Budker Institute of Nuclear Physics in Novosibirsk, who like modern day navvies worked with the installations for several long campaigns.

#### 3 GeV ring

Circumference	528 metre
No. of straight lines 5 metres long	20 pieces
Max current	500 mA
Emittance	< 0,33 nmrad
Beam size, horisontal	40–50 μm
Beam size, vertical	2–4 μm
Horisontal divergens	5–6 µrad
Vertical divergens	1–2 µrad

In August 2015, the installations were completely done and on 11 August 2015, the electrons from the linac could finally be injected into the large ring and 14 days later, electrons were successfully led around the entire 528-metre long ring for the first time without a single corrector magnet having to be activated. This was naturally an important milestone in the project and among other things meant that all magnets were essentially already aligned perfectly from the beginning. The first year was dedicated to being able to characterise and commission the 3 GeV ring and towards the summer of 2016, a maximum current of 175 mA had been achieved, the vacuum system was tested and in the first measurements the uniquely low emittance of the electron beam was confirmed.

It was thereby high time to begin closing the gap for the first insertion devices and continue the work of commissioning the 3 GeV ring in parallel with the corresponding work on the first beamlines. Top-up mode, i.e. injections with closed

#### 1.5 GeV ring

Circumference	96 metre
No. of stratight lines 3,5 metre long	12 pieces
Max current	500 mA
Emittance	< 6 nmrad
Beam size, horisontal	185 µm
Beam size, vertical	13 µm
Horisontal divergens	32 µrad
Vertical divergens	5 μrad

undulator gaps and open shutters that lead to a constant heat load on optical components and thereby better stability, was introduced in June 2017. In September 2018, up to 400 mA could be stored in the ring.

#### The 1.5 GeV ring

Last of the accelerators was the smaller 1.5 GeV ring that on the outside is very similar to the old MAX II ring. It is run with the same energy and has roughly the same circumference as the MAX II ring. It is also somewhat more conventional in its design than the 3 GeV ring. The installations began in May 2015 and were under way for around one year and the first electrons were injected in autumn 2016. The nominal current, 500 mA, was achieved in spring 2018. In contrast to the 3 GeV ring, top-up was implemented from the very beginning.

#### **Operation of MAX-lab**

The old MAX-lab at Ole Römers väg in Lund was in operation with more than ten beamlines during most of the project period and with up to 1,000 users per year. Even if this was naturally a burden to the organisation and meant that a lot of personnel from both beamlines and the accelerator were tied up in operations, the "dark time" in Lund, when no beamtime could be offered to users, was minimised. However, there were no resources for having an overlap between the two synchrotrons so on Lucia Day in 2015, the old MAX-lab was shut down under much ceremony and with the participation of many of those who were involved in the construction and operation of the facility that was successful for so many years.

## Beamline projects *Start-up*

In connection with the positive decision from KAW in July 2011, both the financing and organisation that were to work with the first round of beamlines were in place. Even so, there were very many practical details that were missing, but everyone involved realised that the ambitious goals would not be achieved if these beamlines were to be run as seven independent projects. Projects that compete with each other without coordination and without a desire to find shared



In the beginning of the project the future sometimes looked as unclear as this foggy webcam photo from MAX IV taken 2011, the same day as the first meeting in Yngsjö started.

solutions. However, there was some uncertainty about how to take this further in purely practical terms and what expectations various project participants could have of each other. How should joint projects be identified, prioritised and run and what planning and project tools would be used? To address these kinds of questions the Science Director, all spokespersons, project managers, the project office and representatives of most of the support functions throughout MAX IV gathered at an adequately sized inn and conference centre in the small town of Yngsjö on the north-east coast of Skåne and locked themselves away for a few days. Here, project tools were developed that everyone could feel were relevant and, above all, a mandate and responsibility description for the most important functions in the projects was clarified to a somewhat detailed level. This chance to get away and try to create clarity and consensus in the project organisation was used a few more times during the project period and with the unspoken goal that the talked-about MAX-lab spirit could be replaced with a similar Yngsjö spirit.

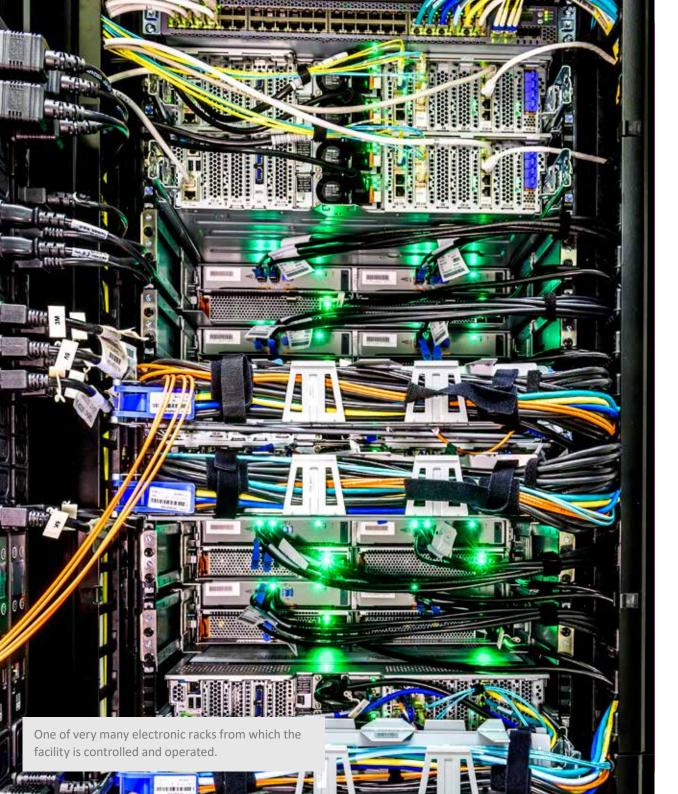
#### Evaluation and international collaboration.

A condition for being able to realise the entire MAX IV project is the help that has been received from experts around the world. It has come in many different ways, ranging from being very organised to being completely informal. Each of the beamline projects co-opted some kind of advisory group, which most often consisted of representatives both from relevant user communities, as well as international beamline experts. Two kinds of slightly special help that the beamline projects received are noteworthy. These are partly the formal external reviews of the design work for each of the beamlines that are implemented around one year after project start. They are done to ensure that the beamlines will perform as intended and are built so that they optimally use the possibilities at MAX IV. The evaluation focuses mainly on insertion devices and optics, which have long production times (12-18 months) and where potential mistakes will be difficult to compensate for later in the project and directly affect the performance of the beamline. Each beamline at MAX IV passes such an evaluation and no procurements in the projects may be initiated before it is complete. The entire process is called the Detailed Design Review (DDR). The project group has to describe the beamline to a detailed level and BPO invites an international group of experts, preferably from other synchrotrons around the world, who go through these details over two days and ask a number of checking questions. This evaluation gave rise to changes in the beamline's design more than once. The process also provides security in the choices made so that progress can continue and the major procurements can begin. An entirely different kind of international cooperation was the agreement set with the Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (BESSY), which is now doing metrology on all X-ray mirrors delivered to MAX IV. These kinds of measurements are a very important quality

assurance and can only be done at a few very highly specialised facilities around the world. As a part of the agreement, personnel from BESSY are also helping to build up the competence in this area at MAX IV. To-date during the MAX IV project, some ten agreements have been signed with other synchrotrons, an indication as good as any other of the importance of this collaboration. MAX IV personnel also made innumerable study visits to other synchrotrons worldwide to familiarise themselves with the details of how they solved certain problems. This was in the same way that MAX IV is now the destination for a large number of study visits from other synchrotrons.

#### Budget and budget follow-ups

Each of the seven beamlines already had separated budgets from the beginning. They would cover hardware and part of the personnel costs (that were not co-financed by MAX IV) during the project phase. The budgets varied between SEK 70 million and SEK 103 million and now at project close, it can be confirmed that overall these budgets, prepared as early as 2010, have held throughout the project. Some activities were somewhat more expensive than assumed at the beginning, mainly the infrastructure, but this was compensated by other activities being less expensive and everyone involved actively trying to reduce costs where possible. In addition, intensive and continuous follow-up work took place throughout the project where the project managers were able to point out deviations from the original budget very early on. The reporting to KAW twice a year



provided further stability in this work. At the end of 2017, the project managers had an opportunity to apply for a co-financing from the surplus from that year in MAX IV's operating budget to cover any negative budget results in the projects. The total project budget for the seven beamlines was SEK 562 million and in this process, SEK 9.6 million in extra grants could be applied for and granted, i.e. less than a 2-per-cent cost increase over particularly complicated projects that have spanned over six years. Good marks for the entire project organisation and particularly for the accounting department at MAX IV under the management of Marie Andersson.

#### Standards and shared solutions

A beamline is very much a jointly built system rather than the sum of a number of individual components. The responsibility rests entirely with MAX IV to both build up the system/beamline and get the individual components to work together as a whole and then operate and maintain them. To manage this with a relatively small organisation, shared solutions that can fit several beamlines must be developed whenever possible. This can be done on many levels. At MAX IV, a number of technical standards regarding multiple areas have grown together. These can concern everything from vacuum components to motor control, as well as seemingly trivial matters, such as adjustable feet that have the same design and are used everywhere regardless of whether they are installed on a vacuum chamber to an X-ray mirror from Japan or a magnet structure to the actual accelerator delivered from Uppsala. This has made the alignment work at MAX IV much easier. Another important standard agreed on was the hard- and software for motor controls. Here, there was also an opportunity to benefit from European initiatives, which means that virtually all motors at MAX IV are controlled through the same motor controller regardless of supplier. Besides these kinds of technical standards, multiple collaborative projects took place on common technical solutions and procurements. Good examples of such cooperation were above all a joint project to develop ultrastable mirror mounts usable at all soft X-ray beamlines in the KAW portfolio and joint procurements of optics for BioMAX and NanoMAX.

#### Support organisations in MAX IV

Of course, it would not be possible to build up these beamlines without extensive support from various parts of the MAX IV Laboratory. It began during the actual design work where the projects got support with very specialised modelling and simulations to find an optimal optic design. On the soft X-ray side, this work was done entirely by Rami Sankari, then active at the Department of Synchrotron Radiation Instrumentation at Lund University. The projects were also given extensive administrative support with the financial reporting and with procurements. Large parts of the projects were also broken out that were run centrally. The insertion devices were one such part where the work was done by a dedicated team under the management of Hamad Tarawneh, regardless of whether it concerned commercially purchased or

in-house developed devices. Design and procurement of front ends rested with BPO while virtually all functions at MAX IV were involved in the infrastructure. Extensive support by many functions at MAX IV was also needed in the actual installations. Electricians, aligners, vacuum and PLC technicians are all examples of functions that had to share their time between beamline and accelerator installations. Lastly, the perhaps largest support counted in man-years comes from the KITS (Controls & IT) group under the management of Darren Spruce that supports everything from motor control to networks, data storage and analysis. In all of these areas, the requirements from the beamlines exploded compared with the beamlines at the old MAX-lab.

This support from the MAX IV organisation naturally does not mean that the project groups can entirely neglect these parts. The projects must still submit their requirement definitions, follow-ups and planning, but at the same time, it provides an opportunity for the projects to primarily focus their work on the areas where they have their unique expertise, meaning the experimental stations.

#### Project closure

The entire project organisation at MAX IV has naturally grown over the years. The project managers have grown in their roles, relevant procedures are in place and necessary coordination and prioritisations take place daily. At the same time, the requirements have also grown. The first beamlines are now entering operation, which does not

however mean that they no longer need resources and coordination. On the contrary, repairs, maintenance and upgrades are needed and will need to be carried out throughout the beamline's entire lifetime. The next generation(s) of financed beamlines have now come so far in their respective projects that they also need major resources from MAX IV in connection with the beginning of their installations. At present, MAX IV is suffering somewhat from growing pains with as many as 16 financed beamline projects under way at the same time, so it is absolutely necessary that extensive coordination and prioritisations are done daily. Some support functions have not been able to expand at the rate that would be desirable and further reinforcements are also needed in the project organisation.

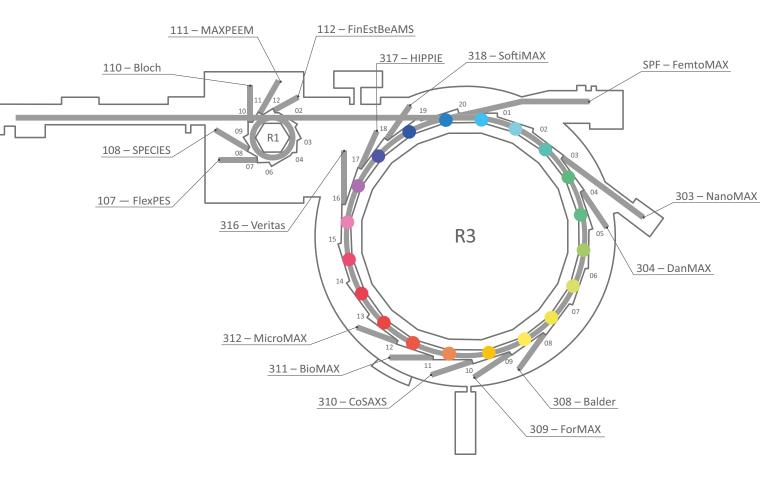
Unfortunately this has also affected the time line for the first seven KAW beamlines. However, today (September 2018), all beamlines from the first wave have had light onto the beamline. Three of them have begun with regular user activities. More will soon follow. However, this does not mean that the projects are completely closed. Alternative set-ups on some beamlines are still being built and all will continue to fine tune parts of the experimental equipment in parallel with the beginning of user activities for a long time to come.

Well, the day that a beamline can be said to be completely finished, it is probably high time to shut it down!

# Beamlines at MAX IV

The 1.5 GeV ring 2015. A large empty space which now is filled with beamlines and other activities.

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Here follows a shorter presentation of the individual beamlines in the first wave financed by KAW and Swedish universities. The texts are based on interviews with the respective project managers.

## BALDER

Balder is a beamline dedicated to X-ray absorption spectroscopy (XAS) and X-ray emission spectroscopy (XES) in the medium and hard X-ray energy range, 2.4–40 keV. The beamline aims to serve a broad user base from material scientists, to geologists, biologists and cultural heritage researchers.

#### By the users, for the users

#### – Katarina Norén

The success of MAX IV will always depend on the users. This was always clear in the minds of the Balder scientists in the development phase of the beamline. All of the inventive ideas and the unique brilliance meant nothing if the beamlines were not attractive to the user community. Like for all the MAX IV beamlines, the scientists from Balder set out early to engage the user community and to solicit input and ideas for their design work. Katarina Norén remembers the initial design phase as very difficult, but talking to users really helped to solidify what was needed and made it much easier to come up with a workable design. When Konstantin Klementiev was brought onto the team in 2013, the Balder project felt like it was well underway. The dialogue with the users did not stop there and, over the years, new design ideas were raised and discussed.

After many talks with the Swedish and German catalysis researchers, it became clear that there was something missing from the original design. That was the ability to do X-ray emission spectroscopy with a high resolution combined with a quick read out. Without hesitation, the Balder team went back to the drawing board and started to work on the design of a spectrometer to be added to the experimental set up. This process was not without a struggle. Changing the specifications of a complex project is never easy and not without an element of risk. However, encouraged by the response from the user community combined with Konstantin Klementiev's innovative ideas, the team re-designed the experimental station and added what was finally called the Scania X-ray emission spectrometer. Like many parts of the MAX IV project, risks were taken but carefully discussed and managed, allowing the potential for a world leading beamline to be made, without ever jeopardising the delivery of a workable solution. The final beamline is today guite different from the initial drawings, but the added spectrometer makes this beamline truly unique.

The Balder team also had a special working relationship with the Soleil synchrotron in France. Joint development with them enabled ways to simplify the beamline optics which made them easier and more cost effective to assemble, leaving scope in the budget for the extra features that the user community needed. The catalysis research community at Chalmers University of Technology also helped a lot, most recently writing grants to introduce diffraction measurements as a secondary technique at the beamline.

Balder, like many of the beamlines, could not have been built without strong internal collaborations with the other funded beamlines which meant that important information was shared and valuable ideas and experiences were discussed. Project planning experience from Thomas Ursby and simulations from Peter Sondhauss were invaluable during the early stages. Close ties were also formed with the beamline teams from NanoMAX, SoftiMAX and CoSAXS to share staff, expertise and ideas for preparing sample environments. At the beginning, the teamwork among the beamlines was about solving technical problems, but as projects become complete this changes, explained Katarina Norén. The challenges are also different, now Balder and indeed the whole of MAX IV is transitioning out of the project phase and needs to become a fully operational facility. This also opens up new possibilities for collaborations. Now the beamline scientists can collaborate with each

Konstantin Klementiev, Lindsay Merte (Malmö University) and Kajsa Sigfridsson Clauss discussing how to best equip Balder to make the users happy.

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other on experiments and user projects where expertise can be shared across beamlines to produce some unique results.

The future for Balder is about delighting the users and getting them to come and use their new machine. This includes users from the old Max-lab, but also new users from different fields such as life sciences. This is where beamline scientists like Kajsa Sigfridsson Clauss have been instrumental and will be even more so as users start coming in. Project manager Katarina Norén explained that the success of Balder has been about finding the right people, assembling them into a working team and trusting them to come up with the best solutions.

#### **Science at Balder**

The medium to hard X-rays at the Balder beamline can penetrate deeply into materials, as deep as a few millimetres or even centimetres. These can therefore pass through windows, capillaries, diamond anvils, etc. into special sample compartments – so called in-situ cells – and thus be used to probe the atomic structure of materials at real conditions, e.g. at high pressures, in a gas atmosphere and at high or low temperatures. The beamline is therefore already predicted to run with a generous amount of different sample environments from the start.

X-ray absorption spectroscopy (XAS) is a local probe of electronic and spatial structure around the atoms of a selected type (elements). Being only element-specific, XAS does not require the samples be crystalline, as opposed to the diffraction techniques. Even more, XAS is applicable not only to solids but to materials in any aggregate state, also to liquids and gases.

Being chemically sensitive and applicable to disordered materials at real conditions, XAS becomes a technique of choice in catalysis research, where hardly any other structural probe can be so informative. Therefore, one of the main application areas at Balder is catalysis. The beamline is equipped with a very complex and versatile gas delivery system, several types of chemical in-situ reactors, analysers of chemical products (mass-spectrometers) and can deliver absorption spectra as frequently as every 100 ms.

One important aspect in applied research is to prepare samples in a well-defined state. However, real-world samples, especially at dynamically changing physical and chemical conditions, frequently represent complex mixtures of several states that are difficult to analyse. Luckily, X-ray emission (fluorescence) lines of different chemical species can often be distinct and the analysis of such emission lines can help in reducing the complexity of absorption spectra. For this purpose, Balder is building a novel X-ray emission spectrometer (Scania-2D) which is currently being commissioned.

Not only chemistry/catalysis will benefit from the installation of the X-ray emission spectrometer at Balder. Environmental research, biology (chemistry of metalloproteins), materials science and preservation of cultural heritage are among the science areas that are expected to be frequently explored at Balder.

#### **Balder**

techniques:	XAS, XES
beam size:	defocused
	V≈0.1–2 mm x H≈2–9 mm
energy range:	2.4–40 keV
time scales:	milliseconds to minutes
samples:	covering K-edges from S to La and L-edges from Nb in almost any sample in any form under many conditions
team members M	ay 2018: Stuart Ansell Konstantin Klementiev Katarina Norén Kajsa Sigfridsson Clauss

The detector has more than 16 million pixels which ensures that the researchers get good data when examining their protein crystals at BioMAX.

XAUIRA

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## BIOMAX

BioMAX is a macromolecular crystallography beamline covering most types of experiments relevant for structural biology including phasing, atomic resolution data collection, high-throughput screening and in-situ crystal diffraction. The aim of BioMAX is to produce a stable and user-friendly beamline that can take full advantage of MAX IV's bright X-ray source.

### Competing around the world

#### – Thomas Ursby

Crystallography is a staple of any synchrotron and the competition to attract users is fierce. Shifts on the beamline are short and the expectations in terms of sample processing and data handling are high. Project manager Thomas Ursby was, however, ready for the challenge when he was appointed in 2011. He had previously worked on the protein crystallography beamlines at both MAX-lab as well as at the ESRF. At MAX-lab he was also in charge of building the beamline. This put him in a unique position, having understood the way the old facility was built and operated, as well has having seen how a new and bigger facility worked in practice. That being said, there was still a lot that was unclear. At ESRF, Thomas was a member of the team building the beamline but here, he needed to build everything from scratch which required a lot of patience. It was similar to the old MAX-lab but on a completely different scale.

For the project team, there was a huge leap to take. At the old MAX-lab, the crystallography beamline had a specific and well-defined niche but at the new facility, they wanted to be the best in the world. It wasn't enough to be technically the best or sometimes the best. The BioMAX beamline would have to consistently perform to the highest possible standard.

Development of beamline optics from the ground up is tricky and laden with pitfalls. For this reason, the team decided to use well established components to build the BioMAX beamline. The rationale was that the beam itself would provide the world leading edge that BioMAX needed and the well-established components for guiding it would provide the stability that the users needed. It would also allow the building process to go faster which was important if BioMAX was to have light before the inauguration in 2016. That is not to say the components included were not the best, for example, the detector for BioMAX is not unique, but is the best model in the world.

Despite the solid idea, the first phases of building BioMAX felt slow, in contrast to working at the old MAX–lab and ESRF. "When users were in and you had a problem, it had to be fixed fast. At the beginning for BioMAX, there was a lot of design work needed and no pressure from users so things felt slow," explained Thomas. The most difficult part of the project has always been the uncertainty.

Developing the infrastructure for the accelerator and the beamlines at the same time can mean that specifications change quite a lot over the months and years. This combined with changing ideas and plans for the beamline designs made it difficult to move forward. Thomas recalled having to decide on the amount of cables needed for the beamline before the designs were completely finalised. However, this feeling disappeared and everything felt more concrete once the contract for the optics was completed in 2013. "It was the first important milestone," said Thomas. Prior to the optics being signed for, it felt like very little in the project was defined. However, with the optics decided, the team felt like they knew what they were working with and progress could continue faster.

The optics arrived late spring 2015, but the time until then passed very quickly and smoothly. Part of this is credited to the internal collaboration that developed between BioMAX and NanoMAX. There were a lot of similarities between the optics and even the detector of NanoMAX and BioMAX which meant they could work together on large parts of the building project and especially with the procurement process which took a long time and was on a larger scale than any member of the team had dealt with before.

In addition to the important collaboration with NanoMAX, the project had great help from the advisory group consisting of representatives from the Nordic user community and experts from some other European synchrotrons. The collaborative spirit that prevails between synchrotrons around the world is also noteworthy, something that everyone benefits from and has been important for BioMAX.

As the old MAX-lab closed the whole BioMAX team could concentrate on the new beamline. New members, including the beamline manager Uwe Mueller, have joined the group since the beamline was funded, now forming a very competent team complementing each other which has made it possible to now be close to completing the full functionality of the beamline as the user operation is ramping up.

BioMAX has a lot of users, arguably the most of any beamline at MAX IV. Paradoxically, the user engagement with the beamline has been relatively low. This is because there are so many users and they spend such a short time at the beamline, that it is hard to be as involved with individual groups as some of the other beamlines are. Unlike some of the other beamlines, the users of BioMAX are not from physics or engineering fields which means they cannot contribute as much to the design and building of the endstation. The users do not have so many specification requirements; they just want it to be of high quality and operational.

The most fun part of the project for Thomas Ursby was 11 days before the inauguration. The team crowded around monitors at the experimental station until late in the evening when the validation of all of their hard work came to fruition. As the team looked anxiously at the monitor, the first ever diffraction pattern from BioMAX appeared to the great delight of Thomas and the team. This was another huge milestone, not only was BioMAX producing experimental data before the inauguration, but they had received first light just two months prior which meant that they had progressed much faster than anyone expected and, indeed, much faster than their international competitors.

Thomas hopes that BioMAX will produce some important scientific results in the future. It is very difficult to say what field it will be in. Structural biology is very diverse and there are a lot of techniques that can be used to study it. However, the field of membrane proteins could potentially have huge implications for the future. These molecules have traditionally been very difficult to crystallise, but high performance beamlines like BioMAX relax the constraints on crystallographers to always produce huge and perfect crystals.

#### Science at BioMAX

Structural biology, in particular macromolecular X-ray crystallography, aims to elucidate the three-dimensional structure of biological macromolecules (proteins, nucleic acids and complexes) up to atomic resolution. The results are providing a basis for understanding all kinds of biological functions like enzyme activity, substrate selectivity, transcription and translation, energy transduction, protein-protein interactions and signal propagation. In addition, structural biology is also an essential component of the method of structure-based drug design used by the pharmaceutical industry. In the last three decades, high-resolution X-ray structures of proteins, DNA, RNA, and biological complexes have revolutionised our understanding of almost all fundamental processes in biochemistry and cell biology. Critical to this development is the use of synchrotron radiation, which has increasingly become mainstream.

More than 90 per cent of all new 3D-protein structures are derived from data obtained at synchrotrons. Synchrotron radiation has had a dramatic impact on the field of structural biology because of the unique X-ray brilliance that can be achieved at synchrotron sources. The parallel X-ray beams of any wavelength obtained from synchrotrons can be adapted to small crystals, allowing more structural information to be extracted from samples of widely varying qualities than would be possible on a home source X-ray generator.

The first macromolecular crystallography beamline at MAX IV; BioMAX, is the newest representative of these international research environments. Here, we are consequently exploiting the unique features of the MAX IV ultimate storage ring to produce a highly parallel, very intense and small X-ray beam, which enables the researchers to run all kinds of X-ray diffraction experiments at this facility. Due to the use of a high automation level combined with high-performance X-ray detector technologies, we are able to collect hundreds of complete datasets from proteins every beam day. This efficiency makes it easier for the researcher to screen through large sample ensembles and find the best diffracting crystal in a short period of experimental beamtime.

In addition, the beamline team in close collaboration with our users, like Richard Neutze's group from the University of Gothenburg, is pushing the limits and is working on the establishment and use of new sample environments for X-ray Free Electron Laser-like serial crystallography experiments. Within this method, we are able to investigate thousands of  $\mu$ m-sized crystals at room temperature and combine partial information coming from each crystal to a complete dataset or even gain experimental information from protein dynamics at a later stage. BioMAX is now ready to be fully utilised by the Swedish and international structural biology community and will certainly soon prove its excellence to our users.

### BioMAX

techniques:	macromolecular crystallography incl. SAD, S-SAD, MAD, atomic resolution data collection, high-throughput screening, in-situ crystal diffraction
beam size:	20 x 5 μm²
energy range:	5–25 keV
time scales:	seconds
samples:	single crystal (1–100 μm) of macro-molecules
team members	May 2018: Ross Friel Ana Gonzales Andrea Gross Gustavo de Lima Uwe Mueller Jie Nan Anastssya Shilova Johan Unge Thomas Ursby

Emil Tykesson, Lund University, checks whether the protein crystals are of sufficient quality to be investigated using BioMAX.

## **BLOCH**

Bloch is the high-resolution angle-resolved spectroscopy (ARPES) beamline at MAX IV and is the evolution of the I3 and I4 beamlines at MAXlab. It is set to be one of the pillars of materials science research at MAX IV, using soft X-rays to understand the behaviour and distribution of electrons in solid materials.

### The workhorse and the show horse - Balasubramanian Thiagarajan

Bloch was initially designed to have two endstations. The idea was that it would be an ARPES workhorse, allowing users to get high quality measurements, as well as having a Spin-ARPES endstation for more advanced experiments. However, the budgeting process in the last stages before submitting the application to KAW required that the Spin-ARPES endstation was removed. ARPES is an instrumental technique used e.g. to understand new, state of the art electronics, which is a field that is constantly changing and growing, and it was clearly important for MAX IV to provide a stable tool for the research community to use. As the beamline team led by Balasubramanian (Balu) Thiagarajan began enthusiastically working on the beamline design, they realised that something was missing.

While the idea of an ARPES workhorse was

attractive, it came with a cost. It had to be stable and relatively conservative which meant losing the ability to be spontaneous and creative with experimental design and sample preparation which had been a hallmark of the I3 and I4 beamlines at MAX-lab. The team became worried that losing this would mean losing what made the beamline special in the first place and losing the spirit of creative problem solving that made the activity at MAX-lab so successful. The question then became, can we create a world leading ARPES workhorse to service the ever-growing demand while retaining our creative freedom?

The answer came from the initial design for Bloch with two endstations. If the original branchline was the workhorse, then the second, Spin-ARPES endstation would be the creative show horse – which would allow users not only to perform Spin-ARPES, but also complementary ARPES experiments, which cannot be done on the first branchline. The beamline team discussed how to produce the spin resolved ARPES branchline that would double the capacity of Bloch as well as give users the chance to explore spin resolved measurements and allow inclusion of creative experiments by providing easy options for flexible sample environment, but without increasing the budget. There was no question that this additional beamline would put Bloch on the map, but perhaps the more pressing question was: should a second branchline even be considered when no funding was allocated for it?

Having no specific funding for a project would have deterred most people but not the Bloch scientists. They started by going back to the designs and specifications for the second branchline. During this phase, Bloch also worked closely with the HIPPIE and Veritas staff who both contributed their expertise from specifications to designs. They then set about recycling and reusing elements from the old beamline, as well as working out how to reduce the cost wherever possible. While this was a challenging process, Balu Thiagarajan was never stressed for which he credits the beamline team (Johan Adell, Mats Leandersson and Craig Polley), the Beamline Project Office for their organisation of the required resources and Burak Kaya for constantly keeping the beamline budget updated. The complexity of the undertaking meant that the whole team had to grow together and to find their own areas of expertise, which they did commendably. During the development, each team member stepped up to take control of critical processes in the design and construction. The encouragement and support from the Science Director, Jesper Andersen with

Mats Leandersson and Johan Adell admires the undulator for Bloch.

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clear indication that the scope and performance of the ARPES branchline is fully maintained was very crucial.

A special mention has to go to the spokesperson Roger Uhrberg from Linköping University. He was responsible for a lot of the external communication and technical discussion for the beamline, without being present for much of the day to day running which presented a significant challenge. Roger Uhrberg overcame this with ease and has been a dedicated and vocal ambassador for Bloch within the scientific community. He was involved as much as possible in the details of the process, often holding the team accountable from afar for decisions and deadlines.

The future of Bloch depends entirely on our interaction with the users. The beamline offers some technical advantages now such as a small spot size allowing measuring of very small samples, but these advantages can be lost quickly as other labs develop similar techniques. Bloch has been designed specifically so that it can be modified and upgraded depending on user expertise and feedback. The hope is that this will be a two-way street. Bloch will encourage an upgrade to help users perform new and exciting experiments, but we will also seek out new users who can teach us how to do techniques that we do not have the expertise to do in-house.

### Science at Bloch

The key to understanding solids and their interfaces is detailed knowledge of the electronic structure near the Fermi level, since this dictates important properties such as magnetism, conductivity, and optical activity. Angle resolved photoemission spectroscopy (ARPES) is a direct and powerful tool to directly measure the electronic structure of crystalline solids, and in particular 2D layers and surfaces. Over the last two decades, ARPES has grown to become a cornerstone of research into novel quantum materials such as high-temperature superconductors, quantum wells, transition metal dichalcogenides, topological insulators and various surface alloys. In particular, ARPES and spin-resolved ARPES have been indispensable tools for understanding graphene (2010 Nobel Prize) and topological phases of matter (2016 Nobel Prize). The rapid growth of ARPES has been driven to a large extent by impressive progress in electron detectors and synchrotron sources, both of which continue to advance at a rapid pace.

The Bloch beamline at MAX IV will provide world class opportunities for preparing novel materials and studying them with a powerful combination of high-resolution spin- and angle-resolved photoelectron spectroscopy, shallow core level spectroscopy, scanning tunnelling microscopy and to a limited extent scanning tunnelling spectroscopy. One of the requirements for ARPES and Spin-ARPES is for the sample to be a single crystal. Many new and interesting materials have single crystal sample sizes ranging from few hundred microns to a few millimetres. The state-of-the-art electronic deflector based DA30 electron analyser, combined with a small light spot size will allow the user community to reliably perform electronic band structure measurements on samples which are very small or consist of multiple domains.

The existence of a second branchline (Spin-ARPES) with complimentary capabilities will expand both the kind of science one can perform and the flexibility for novel experiments. For example, the spin-ARPES endstation at Bloch will have a manipulator exchange chamber on top of the analyser chamber. This particular design was motivated by providing a flexible sample environment, allowing one to adapt the system to explore creative ideas.

Collaboration with groups in Sweden and abroad to exploit the system and also better the system is already taking place. Notable examples include collaborations with Linköping University, Chalmers University of Technology, KTH and Karlstad University. Professor Roger Uhrberg from Linköping University is the spokesperson for Bloch, and has contributed enormously to the design and build-up stage of the beamline. Collaborations with Chalmers University of Technology to modify the STM tip to perform Spin-STM and also for some simple potentiometry measurements is ongoing.

### Bloch

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techniques:	ARPES, Spin-ARPES & CLS
beam size:	10 x 25 μm²
energy range:	10–1 000 eV
time scales:	n/a

samples: e.g. topological insulators, surface alloys, correlated systems, organic molecular layers, magnetic semiconductors, super conductors and other and cooperative phenomena

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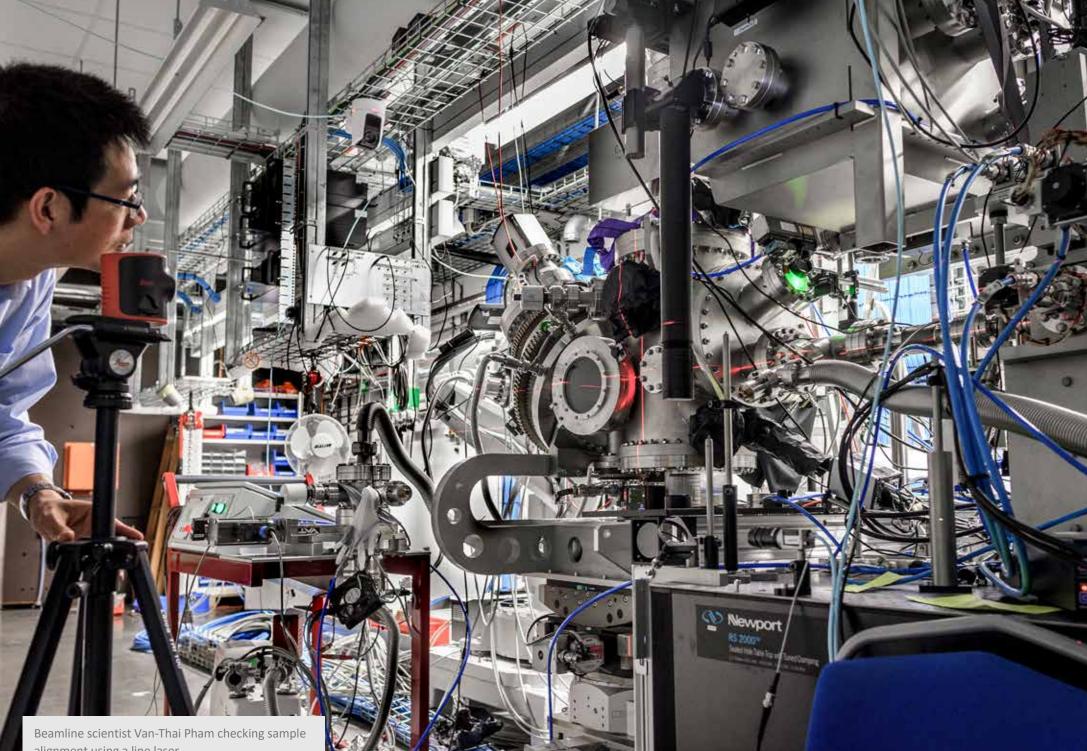
team members May 2018: Johan Adell Mats Leandersson Craig Polley Balasubramanian Thiagarajan

The cryostate at Bloch can cool the samples to about 20 Kelvin, ie. -253 degrees Celsius.

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alignment using a line laser.

### **FEMTOMAX**

A beamline with femtosecond resolution for Time-resolved X-ray scattering, Time-resolved X-ray spectroscopies, Time-resolved SAXS and Time-resolved reflectivity. This beamline is built at the short pulse facility (SPF) at the end of the Linac and resembles a free electron laser.

## Decades of planning for a nanosecond pulse – Jörgen Larsson

Plans for FemtoMAX already existed in 1999. In fact, there was talk about including a FemtoMAX like beamline at the old MAX-lab. "It was better to wait though," said Jörgen Larsson who is the project manager for FemtoMAX. The design for a FemtoMAX beamline at MAX-lab would have meant many challenges that were not present when building at MAX IV which had been designed from the very beginning with a beamline like FemtoMAX in mind. So, despite not having a direct predecessor at MAX-lab, the design for FemtoMAX has been discussed for nearly two decades. This meant that the beamline team were well prepared for the project at hand. They were also very much involved in the beamline D611 on the MAX II ring where many of the time resolved experiments at the old MAX-lab took place.

In 2004, they hosted the first of a series of three workshops. The purpose was to engage scientists

from around the world and to find out what the community wanted from an X-ray beamline with femtosecond resolution. Already in 2007 most of the details of the FemtoMAX beamline were finalised and they "just" needed a new facility.

With the design and specifications of Femto-MAX, it is easy to see how it gets compared to Free Electron Lasers (FELs). There is no denying the power of FELs with their exceptionally peak brilliance, but there are certain niches where FemtoMAX could outperform any of the FELs currently in operation. "This comes from pulseto-pulse variation," explained Jörgen Larsson. In FELs, the pulse-to-pulse variations are very high, which makes interpreting and processing data, often very difficult. This is where FemtoMAX shines. The pulse-to-pulse variation is orders of magnitude smaller than FELs meaning there is a limited loss of data.

In terms of partnership and teamwork, Femto-MAX like each of the other beamlines had a lot of input from external sources. Richard Neutze in Gothenburg advised the team a lot about how a beamline like FemtoMAX could be used to study dynamic interactions in proteins. Willy Sundström from the Department of Chemical Physics in Lund was also instrumental in the design of the spectrometer. These collaborations, along with input from the workshops meant that FemtoMAX also had a lot of input from the user community, ensuring that this would become the best possible tool for users wanting to measure highly time-resolved dynamic interactions.

However, when you examine the collaborations of FemtoMAX within the MAX IV organisation, something stands out. FemtoMAX has only a few scientific collaborations with the other funded beamlines. They are simply too different. With respect to running the equipment and beamline instrumentation, FemtoMAX has a lot more in common with the accelerator division of MAX IV than any of the other beamlines. "They have electrons and we have photons, but otherwise they are very similar," said Larsson.

One of the biggest challenges for FemtoMAX came from the fact that it is so unique. As previously mentioned, they could not take technical advice from the other beamlines, and even though they share many similarities with the accelerator group, the instrumentation is fundamentally different, so there were not many ways to collaborate. The same is true of the FEL community in Europe. FemtoMAX has certain characteristics of a FEL, but it is important to remember that it is not one and as such, the instrumentation and data collection are different. When asked about what was fun about the project Jörgen Larsson replied "we have fun most of the time, building new technical equipment and designing new experiments". It is easy to think that once FemtoMAX is up and running, there will be a lot to miss from the project phase. Larsson has a different view though. He is excited about planning new experiments, and solving technical problems for users but maybe most of all, Larsson is excited about becoming a user himself. All of the work, time and energy going into this amazing piece of machinery make it very attractive to the scientists that built it.

#### Science at FemtoMAX

FemtoMAX facilitates studies of the structural dynamics of materials. Such studies are of fundamental importance for key scientific problems directly related to e.g. programming materials using light, enabling new storage media and new manufacturing techniques; for obtaining sustainable energy by mimicking photo-synthesis; and for gleaning insight into chemical and biological functional dynamics. The X-ray pulses on FemtoMAX have pulse lengths on the time scale of molecular vibrations (100 fs) and wavelengths matching inter-atomic distances (Å). FemtoMAX is a facility for work in several disciplines indicated with the below examples.

Upon femto-second laser excitation, strong changes of the effective potential energy surfaces, which determine the equilibrium structure of a solid, can be induced. This may lead to atomic rearrangement even on a sub-picosecond time-scale. The high flux at FemtoMAX allows for studies of photo-induced phase transitions in solid-matter by diffuse scattering. The ultra-fast macroscopic switching of materials in solid state opens new avenues for the manipulation of matter with light and it will present a high potential for new keys in industrial innovation, e.g. optical information processing (ultra-fast writing and/ or erasing) and optical devices for telecommunication applications (photo-induced refractive index changes). In addition, the (dis)appearance of magnetic species controlled by light (as in spin transition systems) supplies a new channel for information storage.

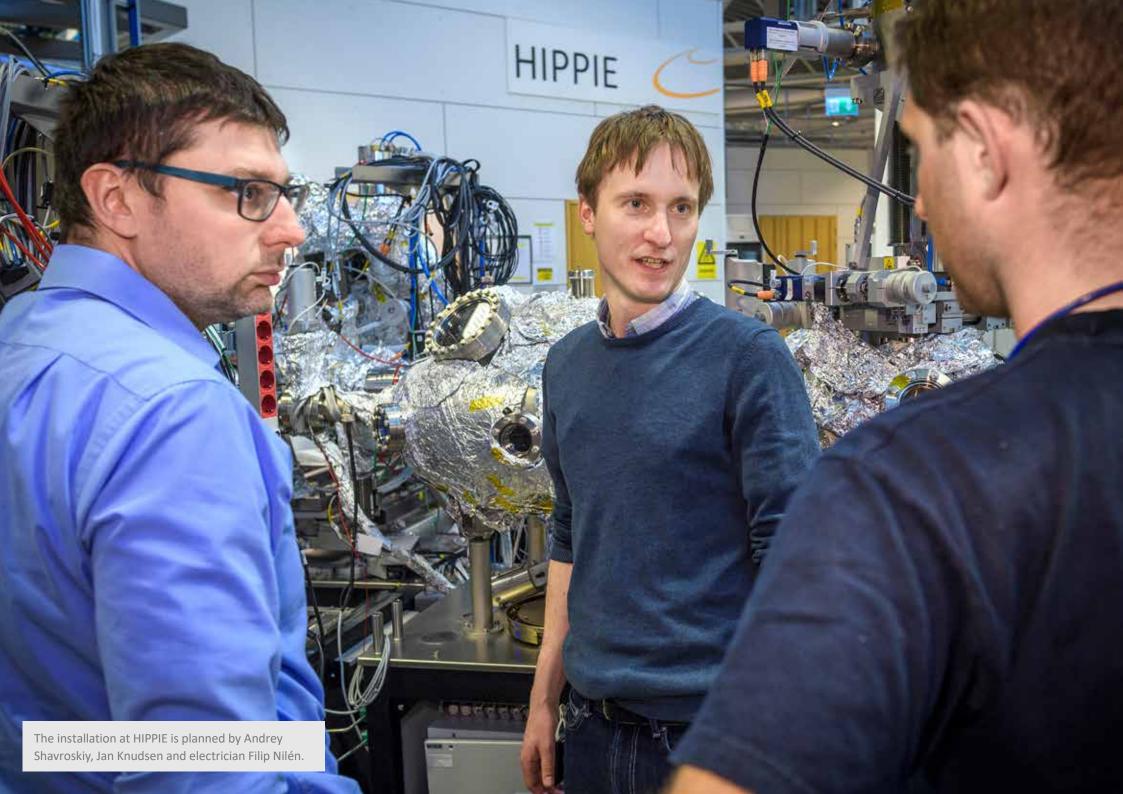
The key reaction steps in many proteins and other biological systems are simple chemical reactions like bond dissociation reactions, bond isomerisation events, and electron transfer reactions, all of which induce conformational changes in the surrounding protein. In solution, these reactions and the coupled solvent response frequently occur on the sub-picosecond to picosecond timescale. In a protein environment, for which billions of years of evolution have optimized the structure for maximum reaction efficiency, the primary photo-chemical events and the ensuing initial response of the protein can be even faster. Photosynthetic reaction centres, the work-horse of biophysics, and rhodopsins, which harvest the energy and information content of light, provide exciting examples of such optimised reactions. Today, various forms of indirect ultrafast optical spectroscopy are the only means to study most elementary steps of biomolecular function. Time-resolved X-ray diffraction and wide angle X-ray scattering (WAXS) experiments at FemtoMAX will allow new experiments and unique structural insights into the function of enzymes and photoreceptors on a time-scale where their remarkable selectivity and efficiency is achieved.

It is a long-nourished dream among chemists to get both structure and dynamics from the same experiment, i.e. to directly obtain time resolved structures showing the three-dimensional evolution of a molecular system in the course of a chemical reaction. There are two routes available to achieve this, time resolved X-ray diffraction and time resolved X-ray spectroscopy. The true molecular timescale, where chemical bonds are broken and formed, charge is transferred between molecules and atoms or ligands are exchanged in the course of a complex reaction, is that of picoseconds and femtoseconds. In order to monitor and follow in real time how such reactions occur we consequently need ultrashort femtosecond X-ray pulses. FemtoMAX can provide the ultimate source for very powerful combined time-resolved X-ray absorption spectroscopy and wide-angle X-ray scattering to yield entirely new insights to the molecular time scale dynamics of electronic and geometrical structure changes and how they are coupled.



techniques: spec	time-resolved scattering, roscopy & reflectivity techniques	
beam size:	unfocused 1 mm diameter; ocused down to 0.01 x 0.04 mm <sup>2</sup>	
energy range:	1.8–20 keV	
time scales: 100 femtoseconds – 100 milliseconds		
samples:	solids (4K–600K), liquids, gases and plasmas	
team members	Andrius Jurgilaitis Van-Thai Pham	
	Jörgen Larsson	

David Kroon and Xiaocui Wang characterize the laser beam which is then used to excite the researchers' samples during the experiments at FemtoMAX.



### HIPPIE

HIPPIE is a beamline for ambient pressure X-ray photoelectron spectroscopy (APXPS). The main goal of the HIPPE beamline is to relax the vacuum constraints that normally apply to XPS beamlines in order to expand the types of experiments that can be performed as well as the user base.

### **Changing phases**

### – Jan Knudsen & Joachim Schnadt

The HIPPIE project team were not strangers to building instruments, or indeed ambient pressure XPS which was used at beamline I511 at MAX-lab. From that perspective, they were more than equipped for the challenge of building the beamline at MAX IV. With that being said, MAX IV was different from any project they had worked on before, both in terms of scale and complexity meaning that there was a lot to learn as the planning process went on.

Like many other projects, HIPPIE relied on strong internal collaboration with other beamlines at MAX IV. Veritas and Bloch were both instrumental in providing support and advice. One of the most difficult things about the project is that it was all new, from the building, to the storage ring and the whole organisation. This meant that there was no template for anything and no good examples to work from and seemingly simple questions, like what should the optics hutch look like and what are the safety implications, could become incredibly complex. This is where the support from Veritas and Bloch became very important as they could address these kinds of questions together, thereby reducing the workload significantly.

The team from HIPPIE also sought advice from the strong XPS community, both in Sweden and internationally. The project then quickly became a living thing, changing and evolving as the needs of the community were discussed and integrated. This led to some of the biggest challenges for the management team. Jan Knudsen who has a keen eye for detail admitted that he had to resist the temptation to micromanage the project which was far too big for one person to oversee every detail. HIPPIE spokesperson Joachim Schnadt had a different challenge. Despite being at Lund University, he found it hard to keep up with the rapid rate of change at the beamline. If he was out of the loop for a week or two, he would find it hard to get back up to speed with everything that had happened.

Facing these challenges ultimately paid off handsomely for the HIPPIE project, making it a truly cutting-edge beamline. One of the biggest changes has to be the electrochemistry setup which has developed into one of the hallmarks of the HIPPIE beamline. Now with the help of international expert and beamline manager Andrey Shavorskiy and Uppsala University, the electrochemistry capabilities of HIPPIE have the user community very excited.

Aiming to be a world leading beamline is not without risk and the HIPPIE project team were well aware of this. Taking and managing risk was part of the culture of MAX-lab. Risk is an inherent part of trying to do things that nobody has done before. "You wouldn't survive if you didn't take risks," explained project spokesperson Joachim Schnadt. While risks were taken, they were always calculated and mitigated. One of the biggest ways of doing this was by finding the right people with expertise that could complement that of the beamline team and help to see problems from different perspectives. "It's important not to clone yourself and just keep doing the same thing," says Jan Knudsen.

That is not to say there were not some tense moments. Jan was always worried that the mirrors would never show up which would have set the project back years. When they arrived, Jan's relief was short lived as the gold coating, which was essential for the function kept falling off. However, Zeiss who delivered the mirrors quickly resolved the problems. The best part of the project to date was when the team saw first light at HIPPIE. It was validation of all the hard work and proof that the obstacles had been overcome successfully. Jan likens the whole process up to this point as a marriage, lots of struggles and challenges before everything works out in the end. Jan also likened the whole process to a marathon. There is no immediate payoff and you have to go through some amount of pain, but then you get something at the end.

Now the team are looking forward to the future and the fun part, doing experiments with their new instrument. They are not the only ones; HIPPIE is at present by far MAX IV's most oversubscribed beamline.

When quizzed about what would be the first big paper coming out from the HIPPIE project the team were philosophical. They explained that, while they had the ambition to publish in journals such as Science and Nature, that is not what the beamline is about. They are here to support the users and the science coming out from HIPPIE now rests squarely on their shoulders. Now, the challenge is to become a productive beamline and to generate new experimental data using the unique features HIPPIE can offer.

#### **Science at HIPPIE**

Many technologically important processes happen in the interphase between different phases. A thorough understanding of the gas-solid interphases is for example essential to obtain an atomic scale understanding of catalytic active surfaces, corrosion of surfaces and growth processes from gas precursors. Similarly, a detailed understanding of liquid-gas and liquid-solid interphases is essential for understanding atmospheric chemistry in aerosol particles and electrochemical processes.

Traditionally, it has been impossible to study such interphases with electron spectroscopies at synchrotron facilities, such as for example X-ray photoelectron spectroscopy (XPS), due to the short mean free path of the created photoelectrons. Recent experimental improvements have, however, lead to dedicated ambient pressure X-ray photoelectron spectroscopy (APXPS) setups that today are in operation at many synchrotrons and laboratories around the world.

HIPPIE is the first APXPS beamline at the new MAX IV facility that went into operation. The beamline and in particular the endstation are designed to fulfil the needs of very diverse user community using different experimental setups. The catalysis cell setup makes it possible to acquire APXPS, infrared reflection absorption spectroscopy and reactivity data simultaneously. It is specifically designed for the study of catalyst surfaces and for general adsorption and corrosion studies in ambient environments. Moreover, the advanced gas dosing system, in combination with the intense X-ray beam from the MAX IV ring and a small cell volume, gives the possibility to work with rapidly changing feed gas composition highly relevant for in-situ kinetic studies of operating catalyst surfaces and atomic layer deposition of thin oxides.

The liquid/electrochemical cell is capable of

performing XPS analysis on liquid-gas and liquid-solid interfaces at equilibrium conditions and under full (photo-)electrochemical control, enabling true operando studies of various energy-related materials and devices (batteries, electrolysers, fuel cells), atmospheric particles (organic, inorganic aerosols), geological formations (minerals, rocks) and biological species (macro molecules to bacteria)

Currently, the beamline staff focus on improving the existing cells and making the complicated setups as safe and user friendly as possible together with software, hardware and safety staff at MAX IV. Future cells planned include: A high temperature treatment cell where it for example is possible to study corrosion of high temperature alloys at idealised gas environment, a cell designed for the studies of biological materials, and a cell designed for the study of membrane surfaces relevant for studies of gas separation membranes and solid oxide fuel cells.

Although the beamline and endstation are focused on APXPS, the beamline staff would like to give users the opportunity to relate to their UHV results, which is crucial for closing the pressure gap between UHV and ambient pressure experiments. This is made possible by the special cell-in-cell design developed at the MAX IV Laboratory, which combines an ambient pressure environment with fully fledged UHV capabilities.

From the expert and first user calls, it is known that the experimental setups offered at HIPPIE are greatly appreciated by the user community. The first articles with results acquired at the beamline have already been published and more will soon follow. The beamline staff are confident that the beamline in its current design will prove itself highly productive in the coming years. They will continue to develop the capabilities, attract new user communities and test and implement conceptually new designs to keep the beamline at the forefront of science.

### HIPPIE

techniques:		APXPS
beam size:		50 x 50 μm²
energy range		310–2000 eV orisontal polarisation)
time scales:		milliseconds – hours
samples:	semiconduct atmospheri	e, catalysis, corrosion, ors, electrochemistry, c chemistry, materials , energy, environment
team membe	ers May 2018:	Jan Knudsen Joachim Schnadt Andrey Shavorskiy Suyun Zhu



### NANOMAX

NanoMAX is a hard X-ray nanoprobe that takes full advantage of the unique properties of MAX IV. The low emittance and resulting coherence combined with diffraction limiting optics produces a highly focused beam allowing for extremely high resolution. NanoMAX can perform a variety of techniques such as scanning transmission microscopy with absorption and phase contrast, diffraction microscopy, XRF (X-ray Fluorescence) and CXDI (Coherent X-ray Diffraction Imaging).

### Unlocking the potential of MAX IV – Ulf Johansson

Of the seven beamlines, NanoMAX is probably the one that exploits the properties of the MAX IV beam the most. The attraction to build such a beamline is that it had potential to be one of the best in the world, allowing experiments to be carried out in Lund that could not have been done before. This lofty goal as well as the novelty of the beamline certainly presented some challenges to the project team. To start with, there was no real user community in the Nordic countries to speak of when the project began. This was something that had to be cultivated as the design and the building project went along. With two workshops, where international experts and the project team began to explain the unique qualities of the beamline, the scientific community gradually became interested. Now NanoMAX has users from many different fields. The expectation was that users would first come from material science. However, the biologists were much faster than expected to adopt the techniques at NanoMAX and they have been very happy with the results.

The emergence of bioimaging at NanoMAX is just one in a whole stack of new things that project manager Ulf Johansson had to learn as he embarked on the journey. Ulf's background was in soft X-rays at MAX-lab, so even the transition to the hard X-ray field was challenging and meant stepping out of the comfort zone. Later recruitments have now also ensured that NanoMAX has a highly skilled team, with complementing competences, supporting the users and the developments at the beamline.

However, Ulf quickly realised that science is only one part in the construction of a beamline. The vast majority is project execution with all of the decisions that have to be made. In this, he found the support of Thomas Ursby from BioMAX to be especially helpful. NanoMAX and BioMAX have a lot of similarities, from the beamline optics, infrastructure and even the detectors. This made BioMAX a good partner to discuss ideas and solve problems with. However, there were some things that Ulf could not be prepared for, such as cockroaches streaming out of the shipment container for the undulator all over the floor of MAX IV, or when the heavy mirror chamber nearly toppled the forklift truck carrying it.

A challenge that arose very early in the design phase was deciding the final length. NanoMAX is the longest MAX IV beamline at a length of around 100 metres as the optics required to focus X-rays to such a small point require space. This in turn meant that the beamline would be too long to be housed within the circular building. However, the exact length was unknown at the beginning as the design for the optics had not been finalised and yet, for the building of MAX IV to continue, the project team had to fixate the length. This was a difficult time in the project phase, but by going through the design and comparing to other beamlines around the world, the team was able to come up with an accurate estimation for the beamline length before building construction began.

The most fun moments of the entire project were when the beam shutter could be opened for the first time and the project team saw light, and a first test experiment could be done just a week before the MAX IV inauguration. When presenting the very first results from the beamline at a conference, it was selected in the conference conclusion



One nanometer is one billionth of a meter, 0.000 000 001 meters. The researchers' samples are mounted on the tip of the small gold-colored sample holder on NanoMAX. Martin Bech, Lund University, assembles a sample at NanoMAX. In the background Tomas Stankevic, Lund University and Alexander Björling (far left) Photo: Ulf Johansson

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as an example of the great achievements and a promise for the future.

The session chair was Ian McNulty who was later to become a Science Director of MAX IV.

In many ways, this symbolised the beginning of the end for the project phase of NanoMAX, although there is still work to be done. User experiments have been done since 2017, simultaneously with commissioning work and remaining project activities. While the project phase will be missed the team is now looking forward to the experiments that can be done at NanoMAX in a beamline that Ulf compares to a Ferrari, "sometimes it fails, but when it works it is quite a fun ride".

#### Science at NanoMAX

X-ray imaging, or X-ray microscopy, comprises a variety of methods for visualizing micro and nanometre sized features with the help of X-rays. With X-rays one is able to see inside a sample without having to open or destroy it, in two and three dimensions, making it a unique tool for many studies. Applications of X-ray microscopy can be found in all major natural science fields, such as materials science, life science, earth science, nanoscience, as well as in other fields of physics, chemistry and biology. Examples of investigated samples are electronic devices, solar cells, lithium batteries, nano sensors, plant- human- and animal-cells, flyash, soil contamination, fossils, artistic paintings, space dust, food, cosmetics, to name just a few.

Questions the scientists are trying to find answers to can be: How many defects are there, shape and size? Elemental composition and quantity? Strain and stress in crystal interfaces? Grain sizes and orientation?

Behaviour of a sample under influence of electricity, heating, cooling and pressure? Differences between samples grown under varying conditions?

X-ray imaging approaching the low nanometre range is one of the most rapidly and strongly developing areas at all modern synchrotrons, e.g., ESRF, Petra3, APS, Soleil or NSLS-II.

A major consideration for the construction of NanoMAX is to utilise MAX IV's exceptional low emittance, high brilliance and coherence properties of the X-ray beam. This will make NanoMAX a flagship beamline for MAX IV, showcasing the full potential of the ring and introducing a variety of new tools for many different research communities in Sweden, as also evidenced by the strong and broad support for the beamline.

### NanoMAX

techniques:	with contras microscopy microscopy diffractic	nsmission microscopy absorption and phase t, scanning diffraction py, X-ray fluorescence (XRF), coherent X-ray on imaging techniques (CXDI), in forward and
		Bragg geometry
beam size:	40–200 nr	m (mature bl ≥ 10 nm)
energy range:	5–24 ke	V (mature bl ≤ 30 keV)
time scales:	n	nilliseconds – seconds
samples:	μm stru devices, frag	us samples with nm to actures, e.g. thin films, gments (earth science, and cultural heritage)
team member	rs May 2018:	Alexander Björling Gerardina Carbone Ulf Johansson Sebastian Kalbfleisch





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### VERITAS

Veritas is the RIXS (Resonant Inelastic X-ray Scattering) beamline at MAX IV. Users will be found from a wide range of different disciplines, but primarily from the material sciences and energy fields.

#### We will learn the truth

#### – Marcus Agåker

It is hard to deny that Veritas is one of the most visually impressive beamlines at MAX IV. The sample sits on a specially designed holder while the detector sits on a huge, 10-metre long arm which is supported by cushions of air and that rotates up to 120 degrees around the sample.

It was a learning process for project manager Marcus Agåker. Building a beamline is not simply about sitting at the bench and building. There are many more tasks that go on behind the scenes such as finding and distributing resources, integrating into the beamline family that is being built at MAX IV as well as developing a strategy for the successful completion of the beamline project on time and on budget. To achieve this, it is important for the project manager to take a step back and allow others to take on the day-today activities of building a beamline. That is not to say the project manager should not be involved at all. Marcus can often be found at the beamline putting things together for Veritas which helps to keep an accurate overview of the project.

The RIXS community in Sweden is quite small, so as the building process came underway, the Veritas team began holding workshops to attract new users. The team tried to understand what researchers in Sweden could do with RIXS and what specifications should be included in the Veritas blueprints. Globally there is a very strong community in superconducting materials that are using RIXS, and it was important the Veritas project catered for these cutting-edge research projects. However, Veritas was also designed to be more flexible and not exclusively optimised for this field. The hope is that more scientists from biology and chemistry will be attracted to apply for beam time at Veritas. By doing this, the beamline will hopefully find a specific niche in the research community as a RIXS beamline that can do experiments like no other.

Marcus Agåker is confident that the key to competing and being successful is the staff at the beamline. This has also been one of the most difficult parts of managing the Veritas project. It was important to rely on the abilities of key people but not so much that the project would collapse if they left. At some point during the project, Veritas had only two staff members compared to other RIXS beamlines that could have many more. This highlighted the MAX spirit that went into building the beamline; doing a lot with little resources. It was also important to convey that this was not a typical academic research project. Timelines and budgets were much tighter than with many other such projects.

Veritas had a lot of collaboration during the project with Bloch and HIPPIE which were the first three soft X-ray beamlines to receive funding. This close collaboration meant that the three beamlines could be proactive about streamlining important development processes such as tendering of common components and the implementation of IT and control systems for the beamlines. Where possible, they tried to organise themselves so that one solution could be developed for all three beamlines at the same time which meant that they got developed faster, but also that resources were saved for other parts of the project.

On the surface, Veritas might look similar to other RIXS beamlines around the world, but it has is an entirely different optical concept and the complete experimental station was designed from the ground up by the Veritas scientists. This design should give Veritas a competitive resolving power compared to other high resolution RIXS beamlines, but it will hopefully also enable the technique to be used on completely new samples. Marcus Agåker has also worked closely with Brian Norsk Jensen from the Stability Task Force at MAX IV to make sure that this was the most stable RIXS beamline in the world.

As the project phase becomes complete, project manager Marcus Agåker sees himself taking a step back. He believes that it is important for others to take on the project and have their input. When managing a project, it is easy to feel a sense of ownership and a need to control things, but in order to be successful, Agåker believes that he must let others come in and breathe new life into Veritas. That is not to say he will be completely absent and that he won't come back to it in the future. Time away and time to reflect are very valuable so that he can return to the project with fresh eyes.

### **Science at Veritas**

The RIXS process is inherently atomic-site specific due to the opening of a quasi-atomic core hole in the first step of the process. The second radiative-decay step ties the atom-specificity to low-energy excited states. These include elementary excitations, which give crucial information about the microscopic origin of materials properties. In addition, the short scattering duration makes the process dependent on dynamics on the femtosecond timescale, which is the typical timescale for interatomic interactions.

The overwhelming potential of the RIXS method is, however, associated with a considera-

ble experimental challenge. To reach the spectral quality, which is essential for fulfilling the scientific visions, the Veritas project exploits the outstanding brilliance of the 3 GeV ring at MAX IV, together with several unique technical developments.

There are especially two fields where improved spectral quality may lead to spectacular advances:

- In strongly correlated electron subtle interactions within the spin, charge, orbital and lattice degrees of freedom give rise to a wide variety of properties and phenomena, including high-Tc superconductivity, colossal magnetoresistance, tunnelling magnetoresistance, multiferroicity and spin-glass behaviour. Elementary excitations reached in the RIXS process include charge transfer, spin and orbital excitations as well as collective excitations such as magnons and phonons, i.e., precisely the excitations that are linked to the property-determining interactions.
- 2. Molecular processes and properties of molecular materials are governed by electronic-vibronic dynamics, which is highlighted in RIXS spectra when the resolving power is sufficient to resolve vibrational excitations. So far only a few such studies have been performed on simple model systems, revealing complex coupling and interactions, especially at intersystem crossings and conical intersections. With improvement of spectral quality, new unexpected opportunities are regularly identified, and it has been demon-

strated that local potential surfaces in large molecular systems can be mapped in a selective way. The science case ranges from basic molecular physics to applications in wet chemistry, including electrochemical process of paramount technological relevance.

While projects at other synchrotrons aim at refinement of the RIXS method for the first case, the Veritas beamline will be unique for the second. The team have given special attention to make flexible sample handling compatible with the high demands on the spectroscopic method.

At Veritas, it will be straightforward to study free molecules in specially designed gas-cells, interactions in liquids in microjet setups, molecular materials with innovative methods to avoid radiation damage, and processes in in-situ and in-operando cells.

#### Veritas

techniques:	RIXS
beam size:	1 x 5 μm
energy range:	275–1500 eV
time scales:	seconds
samples:	materials science, correlated systems and energy materials
team members May 2018:	Marcus Agåker Shih-Wen Huang Conny Såthe Nial Wassdahl

Seeking the truth requires focus. Refocusing mirror at Veritas.

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# THE USERS – OUR RAISON D'ÊTRE

Jesper Wallentin - synchrotron scientist through stipend from KAW

Despite the history and pedigree of MAX-lab stretching back to the mid-1980s, MAX IV was completely different. Just before the royal inauguration, Sweden was about to be thrust onto the world stage with a facility that would rival the best



synchrotrons anywhere on the globe. In doing this, there was a risk that there were not enough Swedish researchers with the experience needed to use such a powerful machine. Building a brandnew research infrastructure is not only about cutting-edge equipment, it is about developing researchers who are well positioned to use it.

A perfect example of this is the story of Jesper Wallentin, a solid-state physicist turned synchrotron physicist through the incentives and guidance of KAW.

Jesper finished his PhD in solid state physics and was attracted to a stipend call by KAW for synchrotron physicists. The idea was that Jesper would spend two years doing postdoctoral research in a foreign lab doing synchrotron physics before coming back to Sweden. On his return to Sweden, Jesper would be expected to find funding for a position at a university, but crucially, he would have financial support from KAW if he needed it. This generous funding scheme not only allowed Swedish researchers to get the training they needed, but also gave them the security to be able to establish themselves at Swedish universities and strengthen the whole field of synchrotron physics.

Jesper received the funding and moved with his family to Göttingen, Germany to work with Tim Salditt, who is an expert in X-ray imaging. While working there, Jesper became interested in developing methods for imaging nanowires and crystals which is an important technique for the NanoMAX beamline. Now, he has a position at the Faculty of Science, at the division for Synchrotron Radiation Research. While he did not need the full amount of funding from KAW, it was an important safety net that allowed him to focus on finding a position and doing world leading research.

His work now focuses on developing sample environments to study nanomaterials. This

means that his results can have huge knock-on effects for the beamlines and for users.

#### Calls for proposals

So far, five calls for proposals have been published since the start in 2016. The first three KAW beamlines, BioMAX, NanoMAX and HIPPIE, currently receive regular users while the first experiments with expert users who assist in the commissioning of the beamlines have already been implemented or are on their way for the other KAW beamlines. The first call for regular users for six of the KAW beamlines plus two additional beamlines on the 1.5 GeV ring will be published in spring 2019. Most applications come from Swedish universities and organisations, but the facility attracts users from all over the world just as MAXlab did during the years it was in operation.

The interest from the users is sizable, and several of the calls for proposals that have been published have generated many more applications than the beamlines have been able to receive. The process of selecting which applications are to be offered beamtime at the lab is led by the so-called Program Advisory Committee (PAC). These committees consist of internationally renowned scientists in each specific field of research, and their task is to select the applications that are of the highest scientific level and which can best use the brilliant synchrotron light produced at MAX IV.

A challenge for MAX IV is to arouse the interest of new user groups, researchers who have never before come into contact with synchrotron lights and who therefore do not know how it can contribute in their research. Some research fields in which this work is now in progress are forest and pulp, food and environmental research.

In this work, both the User Office, Industrial Relations Office and the spokespersons and radiation pipe managers are essential but also FASM - The Association for Users of the Synchrotron Light at MAX IV - plays a significant role. Not least because FASM is responsible for the annual user meetings where the researchers meet and exchange experiences and ideas for future research at the facility.





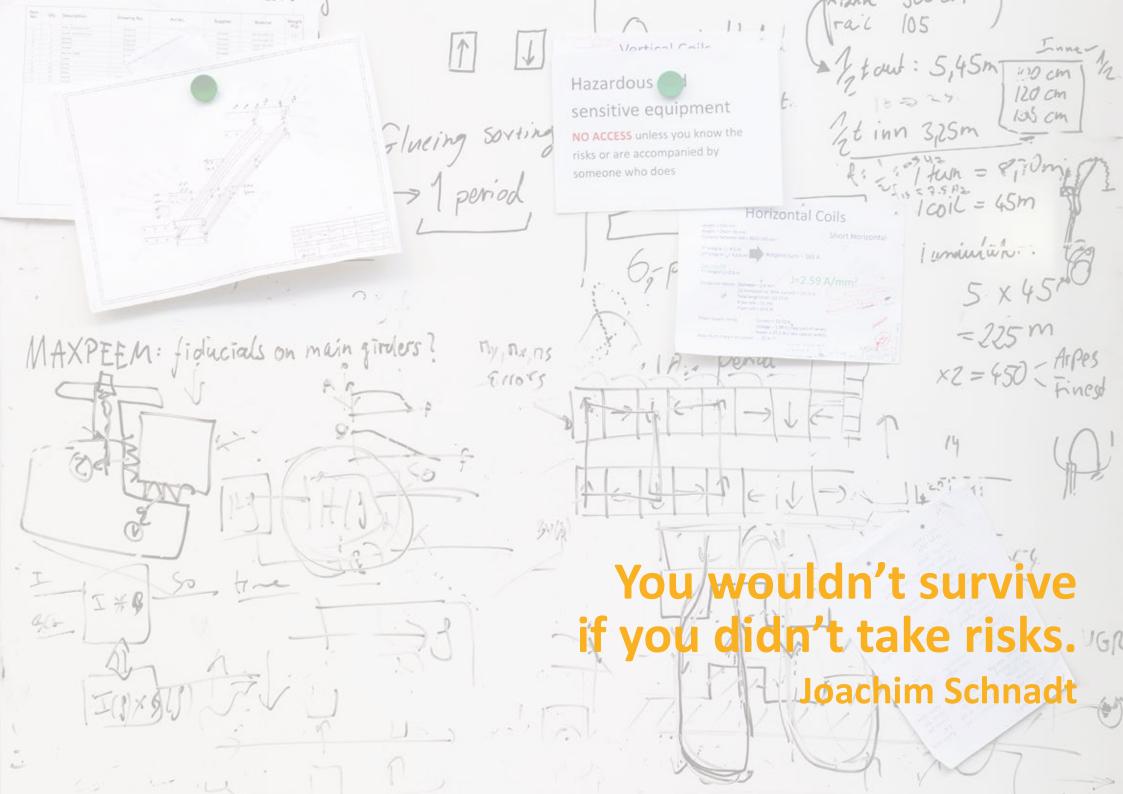
Christian Disch, Dectris och Jörgen Larsson testing a Pilatus 3 detector in Time-over threshold mode enabling counting several photons in each pixel and shot.

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Marianne Liebi, Chalmers, and Ulf Johansson, MAX IV, are satisfied with the results from NanoMAX. Photo: Tomas Stankevic.



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