ANNUAL REPORT

2023

MAX IV

MAIN FUNDERS AND PARTNERS

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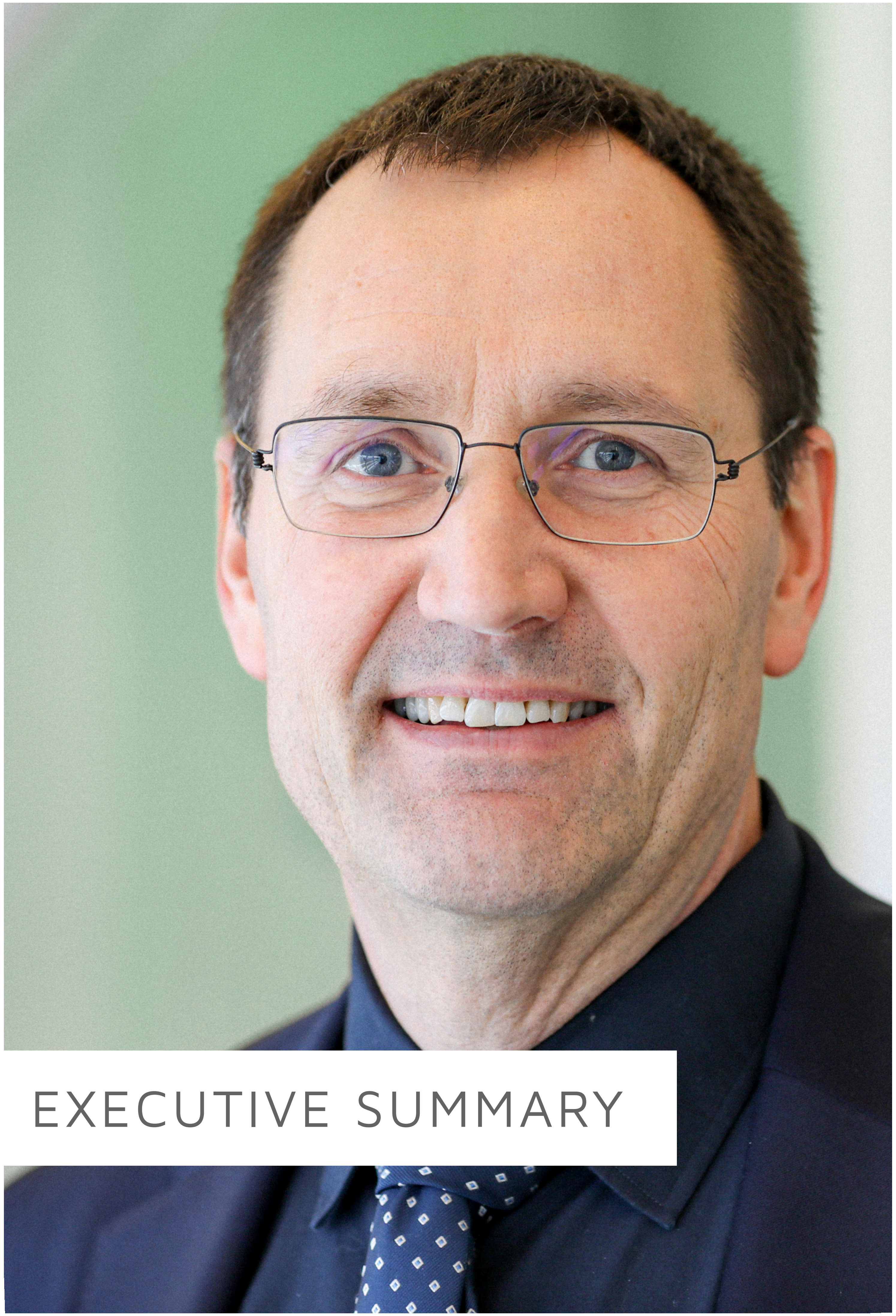


EXECUTIVE SUMMARY

Dear MAX IV community,
You are now reading the first version of MAX IV's Annual Report in a new format. We have attempted to show a comprehensive picture of the user science and MAX IV during 2023 and give you insights into what we aspire to accomplish in 2024. We hope the report will provide you with both valuable information and enjoyment.

In 2023, our users conducted more than 300 scientific projects at MAX IV. The results of these projects range from applications in everyday products to foundational research that addresses future challenges. The opening of all 16 funded beamlines for User Operations was a significant achievement towards realising the vision outlined in our Strategic Plan 2023–2032.

Our roadmap includes the development of three Conceptual Design Reports for new materials science beamlines, a collaborative effort with the Wallenberg Initiative Materials Science for Sustainability (WISE). Our growing partnership in medical imaging will result in a conceptual design report for an imaging/tomography beamline with in vivo capacities at MAX IV. To maintain the competitiveness of our existing and future beamlines beyond 2030, our Strategic Plan includes an upgrade to the 3 GeV ring – MAX 4^U – that aims for significant coherence and brightness improvements.

Organisational milestones in 2023 were the establishment of our Technical Division and the recruitment of an Administrative Director. These have enhanced our capabilities, allowing us to support our expanding range of scientific endeavours better and improve our internal processes. 2023 also brought a new period of leadership for MAX IV with the welcoming of a new Board on January 1, chaired by Robert Feidenhans'l, and my transition from interim to full-time Director of MAX IV.

Throughout the year, we have received crucial support from our Board and advisory bodies – the MAX IV MAC (Machine Advisory Committee), PAC (Programme Advisory Committee), SAC (Scientific Advisory Committee), and URG (University Reference Group). Thanks to their invaluable insights and guidance, we were able to make significant progress in our development.

During Sweden's Presidency of the Council of the EU, MAX IV participated in the EU meeting in Lund in June 2023. The meeting highlighted the importance of high-quality research data, responding to crises, and emphasising Open Science practices. Distinguished keynote speakers, including Mats Persson, Minister for Education, underlined the foundational role of research infrastructure in addressing complex global challenges.

MAX IV has marked a growing interest from industrial users. While most industry-related research is conducted in collaboration with academia, there are several initiatives in progress to make it easier for less experienced companies and business sectors to get involved. We have also initiated collaborations with experts in data analysis and impact assessment to enhance our ability to quantify and monitor our societal impact goals. We hope to share these insights with you in 2024.

This year also posed significant financial challenges, particularly with increased costs of electricity and rent. However, we have received financial guarantees from our hosting organisation, Lund University, which has been crucial to arrive at an approved budget. Additionally, the Swedish Government provided supplementary funding for 2024 in September. Although it does not cover all our needs, it is a significant gesture of support and reflects Sweden's commitment to maintain a leading role in science and technology. With strong support for MAX IV in our community's inputs to the research bill, we anticipate improved long-term financial stability starting in 2025.

Thank you for your steadfast support and relentless curiosity. Together, we are committed to enabling world-class science for a brighter future.

Sincerely,

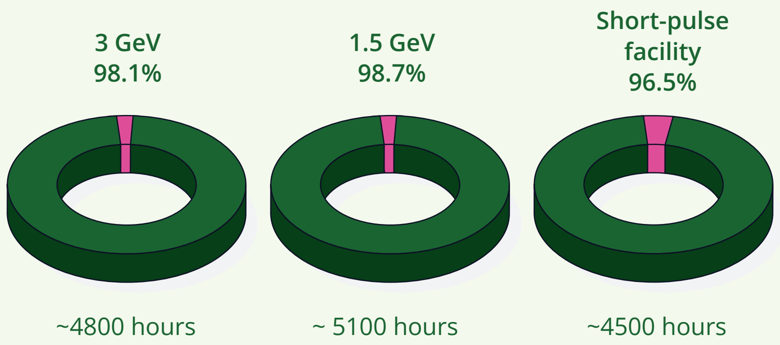
Olof "Charlie" Karis
MAX IV Director

FACTS & FIGURES

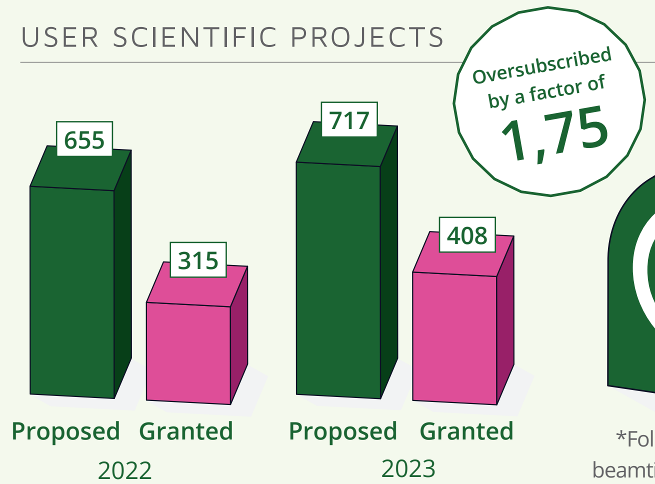
BEAMLINES

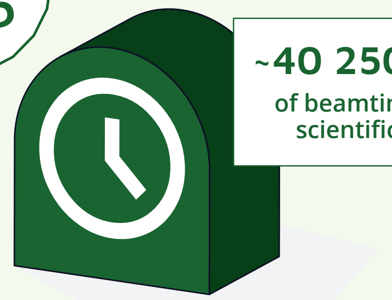
In 2023, MAX IV's 16 beamlines were open for proposals for the first time. Continuous developments resulted in the addition of various technical capabilities at the beamlines. Three conceptual design reports (CDR) were established with the user communities for potential developments of new beamlines to support research for materials science for sustainability.

ACCELERATOR UPTIME



USER SCIENTIFIC PROJECTS



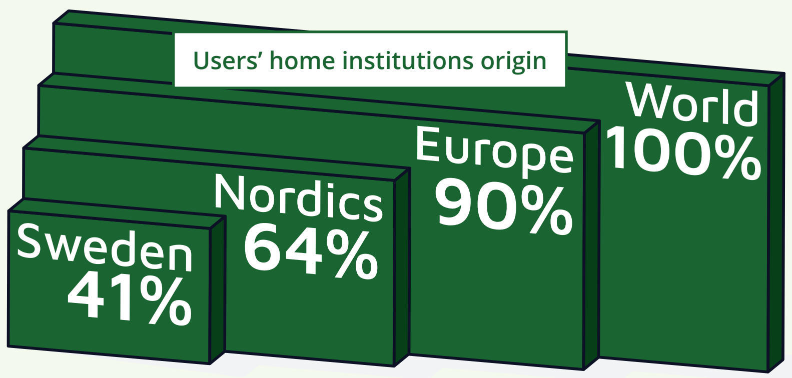


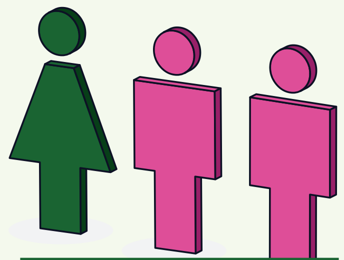
~40 250 hours*
of beamtime for user scientific projects

*Following the Swedish Research Council's definition of beamtime hours, based on cycles, including proprietary use.

USERS

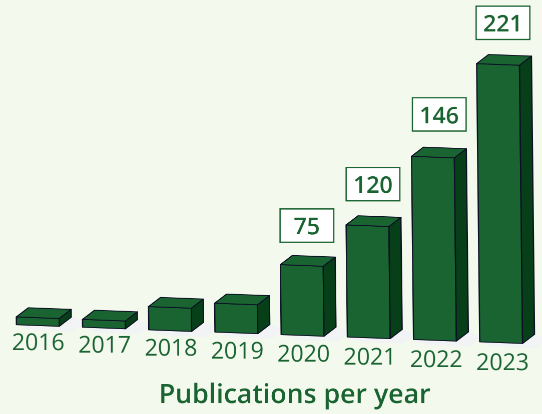
1732 unique users from **280** institutions across **34** countries out of which **14.7%** remote users





1 in 3
users is a female scientist

PUBLICATIONS



+51%
increase of publications compared to 2022

651
publications 2016–2023

RESEARCH AREAS

- Physics and astronomy
- Chemistry
- Chemical engineering
- Materials science
- Engineering
- Energy
- Life and health sciences

INDUSTRY

23 proprietary user groups including mediators

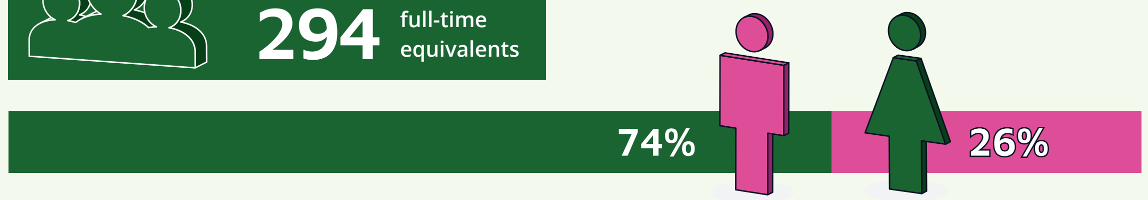
52% proprietary industry users from Sweden

~4950 hours
of beamtime for user scientific projects connected with industry

~850 hours
paid proprietary beamtime

EMPLOYEES

294 full-time equivalents



SUSTAINABILITY AND ENVIRONMENT

As a world leading synchrotron research facility, MAX IV works on progressive measures to demonstrate commitment to a better, more sustainable future. The facility works to ensure that its operations and organisation contribute to positive environmental, societal, and economic impacts on both local and global levels.

MAX IV's Strategy and Roadmap state that the facility's organisational conduct, projects, and operations should consider impacts on the environment, people, and climate. Thus, MAX IV employs a continuous and dynamic process to ensure its goals within sustainability are achieved.

Upon the completion of the MAX IV Strategy 2023-2032, a sustainability task force was created to give laser-focus attention to sustainability work at the facility. The group is comprised of various team representatives tasked with a strategic mission to compose an original sustainability plan for MAX IV. MAX IV is taking responsibility to contribute to the United Nations global goals, not only from research output and infrastructures, but also operation. The sustainability plan covers various aspects of sustainability and demonstrates the organisation's commitment to positive relationships with surrounding communities and stakeholders. Through collaboration the facility's resilience and competitiveness will continuously increase. The sustainability plan will be finalised in 2024 and implemented facility-wide as soon as possible. The plan will be updated, reviewed, and recalibrated bi-annually.

Sustainability work at MAX IV is guided by the UN Sustainable Goals, particularly through science and research work at MAX IV. On the operational side, several goals have been prioritised, including high-quality education (4), affordable and clean energy (7), industry, innovation, and infrastructure (9), sustainable cities and communities (11), responsible consumption and production (12), climate action (13), partnership for the goals (17). While MAX IV's efforts address additional goals, it strives for impact in these focus areas.

THE GLOBAL GOALS
For Sustainable Development

Figure 1: The 17 Sustainable Development Goals (SDGs). On the operational side, MAX IV has prioritised several goals, including number 4, 7, 9, 11, 12, 13, and 17.

At the buffer system that helps securing toxic gas waste in the facility.

Research

From atmosphere and climate to wood at the molecular level – research for sustainability at MAX IV is conducted continually. Scientists come to MAX IV on a mission to explore sustainable solutions. Beamlines at MAX IV are equipped to assist scientists in uncovering the knowledge gap. MAX IV is involved as an organising partner or collaborator within projects involving sustainability research solutions such as PRISMAS and ReMade.

ForMAX beamline, for example, is dedicated to advanced studies on wood-based materials. It allows in-situ multiscale structural characterisation from nanometer to millimeter length scales by combining full-field tomographic imaging, small and wide-angle X-ray scattering (SWAXS), and scanning SWAXS imaging in a single instrument. ForMAX focuses on research of new, sustainable materials from the forest, but also allows for research in many other fields and industries, including food, textiles, and life science. In 2023, the beamline officially opened for experiments and welcoming users conducting research on sustainable materials.

In 2023, MAX IV also conducted a series of workshops in collaboration with WISE (Wallenberg Initiative Materials Science for Sustainability) to develop conceptual designs for three potential materials science beamlines. The conceptual design for the beamlines is being developed and defined together with the Swdish scientific community. The collaboration is entering a new phase in 2024.

To promote sustainability research from industrial users, the laboratory will assume the role of facilitator. MAX IV works to engage industrial users to reach the UN Sustainable Development Goals. To achieve this, sector-based initiatives targeting the ten industry sectors of strategic interest in the Nordics are prioritised.

The latest updates on sustainable research at MAX IV are communicated via the website and facility reports.

Climate

MAX IV is committed to long term environmental sustainability efforts and conscious reduction of the carbon footprint. Therefore, it is vital to continually measure critical factors that affect our environment in relation to daily operations. The high-level research done at MAX IV requires an intensive level of energy, but through engineering technology and innovation, the facility requires significantly lower energy to operate as compared to similar synchrotron facilities globally.

Since 2016, MAX IV's energy consumption has increased gradually during the transformation into an operating facility. However, even with the growing number of beamlines, MAX IV has successfully limited electricity use facility-wide to the point where it effectively leveled over the last several years.

Before 2024, MAX IV invested 2.9 MSEK in energy efficient solutions that will ensure long-

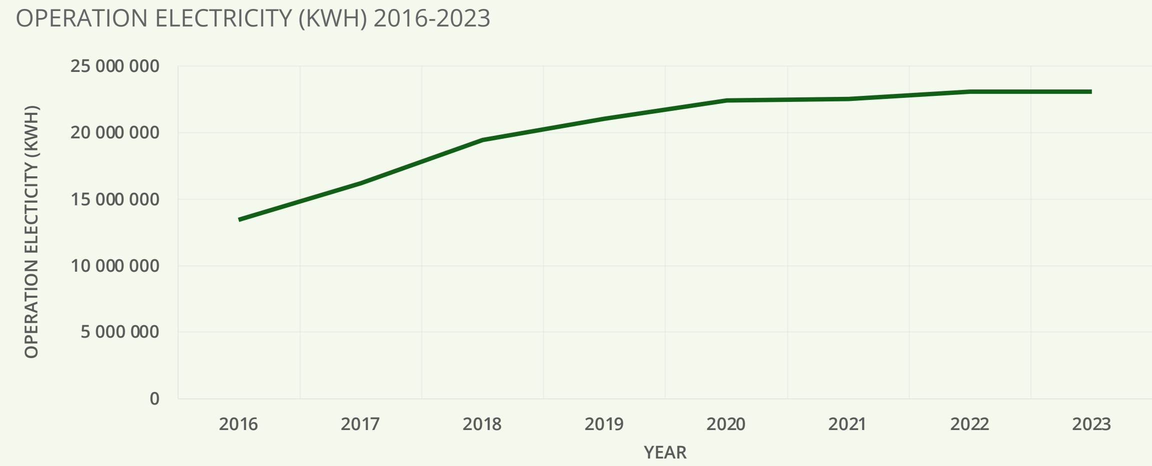


***Figure 2:** MAX IV energy consumption 2016-2023.*

term gains. A project plan to invest an additional 2.3 MSEK in energy efficient projects is ready for implementation during 2025-2027, which is estimated to save 2.5 MSEK annually once concluded.

The MAX IV facility is equipped with solar panels on the office buildings, controlled ventilation, and motion detected light fixtures. Collaboration with the energy company Kraftringen enables the reuse of heated water in the world's largest low-temperature district heating network in the city of Lund, where MAX IV is located. To ensure efficient energy use, MAX IV's Facility Management team created an energy efficiency report in 2023 which identified the most impactful areas to focus efforts towards efficient energy savings. A facility-wide collaboration is currently underway in 2024.

Learning from the COVID-19 pandemic, MAX IV will continue to provide opportunities for remote or hybrid experiments contributing to reduced commuting for scientists who previously needed to be physically present onsite. These modalities help reduce carbon emissions from travel. Remote and hybrid access are offered at many beamlines to a varying extent, with BioMAX primarily operating in full remote mode.

MAX IV has implemented a mobility solution since the relocation of some staff to the MAX IV Cube office. Staff have free access to public transportation to commute between the Cube and the MAX IV main facility (Fotongatan) on work-related business. To complement this, 25 bicycles are available for use to commute between the sites.

Since 2023, MAX IV also participates in CoAction, a joint cooperation led by neighbouring neutron source research facility ESS to find new possibilities to reduce goods transports to our facilities. CoAction aims to find opportunities to coordinate freight flows between ESS, Lund University and MAX IV to be efficient and not produce unnecessary CO2. The project will last until 2027 and includes many different work areas such as procurement, gas deliveries and waste pickups.

Waste management

In the years since MAX IV moved into operations phase in 2016, the general waste and hazardous waste volume has steadily increased. In 2023, general waste sorting of recyclable materials improved significantly while also reducing the number of containers for residual waste. More efforts are aimed at waste mapping, investment in waste compactors, purchase of alternative or recyclable items and availability of recycling facilities in the building. MAX IV will work to implement these improved changes in the remaining areas during the next years. Routines for waste handling have been improved. Internal informative sessions have been held, such as presentations at facility meetings, and information disseminated through internal newsletters.

Food and conferences

MAX IV regularly purchases coffee, tea, chocolate powder, milk for coffee machines and fruit for employees. In 2023, 81% of the food and beverages procured by MAX IV was organic (KRAV alt. EU organic) and Fairtrade labeled. MAX IV will continue to follow the goals and activities of the sustainability plan when ordering catering and food. By using sustainability criteria in procurement and participating in Fairtrade City Lund, MAX IV works continually to reduce environmental impact. The organisation also follows Lund University's policy stating vegetarian food should always be the first option at any catering or dinner events.

Building management

The MAX IV building was constructed with sustainability in mind. Its operations are certified in accordance with BREEAM Outstanding standards, "Green Building" and Miljöbyggnad Guld due to the high environmental standard. A comprehensive programme for the building's life cycle exists to cover construction, operation and maintenance, and future demolition of MAX IV.

The construction process itself included "greener" logistics, low energy consumption, minimal waste, waste management, installation of LED lights in all buildings, and more. Controlled ventilation and green roofs improve insulation and help stabilize the temperature in the experiment hall.

MAX IV encourages continued support for biological diversity by maintaining the surrounding land as a green area. The space is planted with a mix of seeds from nearby nature reserve, Kungsparken. The facility also manages the building and maintenance of rainwater ponds with wetland vegetation to sustain vulnerable and threatened species. These nature-based solutions are designed to also store and delay storm water from both annually recurring storms and once-in-a-century storms to reduce the impact on wastewater systems and imrpove wildlife environments. MAX IV has also erected a 'bee hotel' to assist wild bees in finding suitable hibernation areas.

Chemical safety

Many different types of hazardous waste are produced at MAX IV in small quantities. Oil emulsions from old machinery, various types of laboratory chemicals for research preparations and cleaning agents are the main hazardous waste produced. The decrease in hazardous waste during 2021 is due to reduced operations during the COVID-19 pandemic. Improvements were made in 2023 to significantly reduce the amount of hazardous waste produced in the workshops. The workshop upgrade constitutes an increased amount of lubricant hazardous waste in 2023, however this will be a one-time occurrence.

MAX IV continually works to reduce incidents caused by improper handling of hazardous waste.

Hazardous waste management has improved through implementation of updated procedures and routines, lab access training modules, and targeted information for users and staff. With this implementation, incidents concerning hazardous waste have reduced significantly compared to previous years.

To increase user and staff awareness for sustainable handling of lab equipment, MAX IV implemented lab access training. The training includes information on safe and sustainable handling of lab equipment, chemicals, and waste. The training is obligatory for users and staff who access to the preparation labs. The number of training courses increased over 500% in 3 years. The increase is closely related to the increasing number of beamlines beginning operation. One training course can include 1-5 people. MAX IV continues to work towards environmentally sustainable procurement of lab equipment and PPE (personal protective equipment).

LABORATORY EDUCATION 2020-2023

Figure 3: *Preparation lab training sessions conducted for users and staff 2020-2023.*

Close-up of the green roofs at MAX IV which improve insulation, help stabilising the temperature in the experiment halls while storing and delaying rainwater drainage to reduce the impact on sewage systems, and improve wildlife environment.

Procurement

MAX IV strives to meet sustainable procurement requirements that includes environmental, social and economic sustainability. MAX IV ensures that energy utilised is procured from a sustainable and renewable source in accordance with EUs taxonomic definition.

The Public Procurement Act and The National Agency for Public Procurement (Upphandlingsmyndigheten) stipulate that sustainability requirements be used in all procurements work. Procurement aspects are an important part of the Lund University sustainability plan. The university's goal is to use sustainability requirements at a basic level in all procurements, where possible. When relevant, ISO standards or equivalent are required from suppliers.

Computing and IT infrastructure

Aligned with Lund University guidelines and sustainability goals, MAX IV works efficiently regarding electronic procurement and electronic waste management. Procurement contracts, based on Lund University' procurement regulation, require suppliers to fulfill government-regulated standards which consider the environment and sustainability. A new Lund University policy on the recycling of IT equipment designates the reconditioning and resale of equipment before recycling.

On the operational side, the accelerator and beamline control are run in virtual machines, thereby reducing the number of physical machines leading to a much more efficient use of resources. The cooling of the server halls is done via the same cooling water system used by the accelerator, which returns heat to the common heating system for the nearby neighbourhood of Brunnshög.

USER SCIENCE PROGRAMME

FOREWORD

In 2023, the number of unique users and beamtime hours awarded to academic users through Open Calls both grew by approximately 31% compared to the previous year. 834 hours of proprietary beamtime were sold. The user base is growing rapidly and MAX IV is expanding its offerings at a fast pace.

While the total number of beamtime hours used in 2023 was 40250, the beamtime awarded to academic users through Open Calls increased from about 27400 in 2022 to nearly 36000 in 2023. This indicates an intense development phase, where more beamlines are coming online, and existing beamlines evolve and reach new user groups. Three main beamline construction projects were completed at ForMAX, CoSAXS, and NanoMAX, and more beamlines added capabilities from beamline operations funding.

Compared to MAX-lab (1987-2015), MAX IV has nearly tripled its Swedish user base (users affiliated with a Swedish home institution) as a driving force in Swedish synchrotron science. According to statistics, MAX IV is the most important facility for the Swedish user community, and it is expected that this will be reflected in publication data over the next 3-5 years.

Although the Swedish utilisation of MAX IV increased in 2023, the growth rate was slower than in previous years, while the international utilisation of MAX IV grew faster, particularly by first-time synchrotron users. The increased international recognition MAX IV has gained for its competitive beamline performance and scientific relevance has contributed to the growing popularity among user communities.

USER SCIENCE PROGRAMME UPDATE

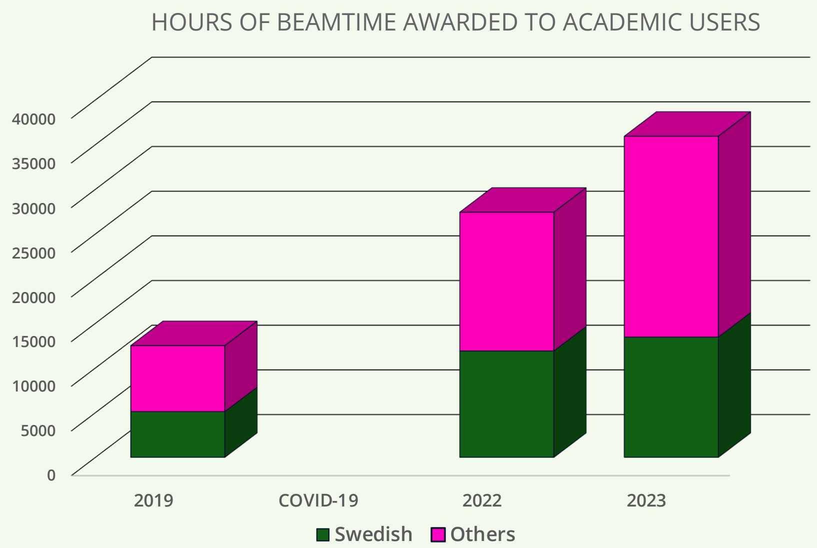
The number of unique users increased by 31%, from approximately 1300 in 2022 to more than 1700 in 2023 (see Figure 3). The growth in external researchers using MAX IV is a testament to the increasing capabilities and the attractiveness of the User Science programme. Currently, MAX IV has 80% more users out of which 70% more Swedish users (affiliated with a Swedish home institution) than the MAX-lab facility had at its peak in 2015. This means that MAX IV has nearly tripled its Swedish user base compared to MAX-Lab.

In 2023, more than half of the researchers who utilised MAX IV had not used it since its inauguration in 2016. They were either new members of established user groups, such as PhD students or postdocs, or entirely new user groups, demonstrating that MAX IV is attracting a rapidly growing user community. The statistics also reveal that MAX IV is a Swedish facility with a strong Nordic user base. 64% of the users (around 1100) are affiliated with Nordic home institutions, of which 41% (around 700) are affiliated with Swedish home institutions (see Figure 4).

The beamlines have continued to improve and showcase world-class performance, leading to increased international recognition. Reflecting this, the percentage of international users has grown faster than the relative percentage of Swedish users in the last two years (see Figure 3). In 2023, the percentage of Swedish users was 41%, which is slightly lower than the range of 42.5% to 44.6% at the old MAX-lab facility between 2012 and 2015.

It is worth noting that about a fifth (20%) of all beamtime was used by multinational groups comprised of users from different geographical home institutions.

Figure 1: Beamtime hours awarded to academic users through the open calls in 2023, scheduled for the second half of 2023 and the first half of 2024. The percentage of hours awarded to Swedish academic users for these years was 41% (2019), 43% (2022), and 37% (2023). No comparable data is available for the pandemic years (COVID-19, 2020-2021).



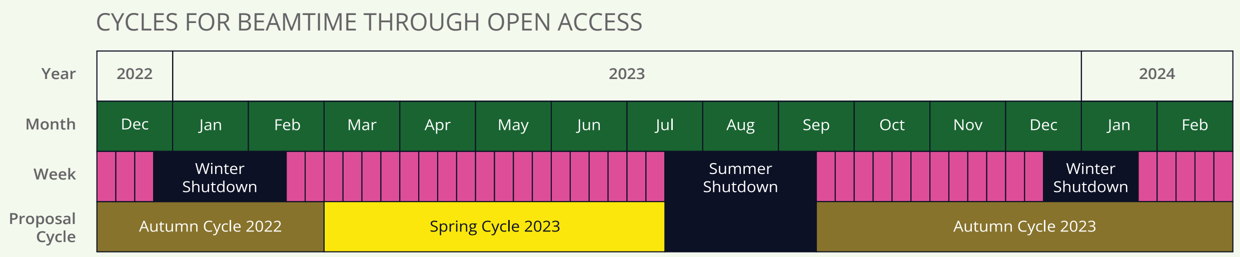


Figure 2: Cycles for beamtime through open access in 2023, named according to the scheduled beamtime period and year.

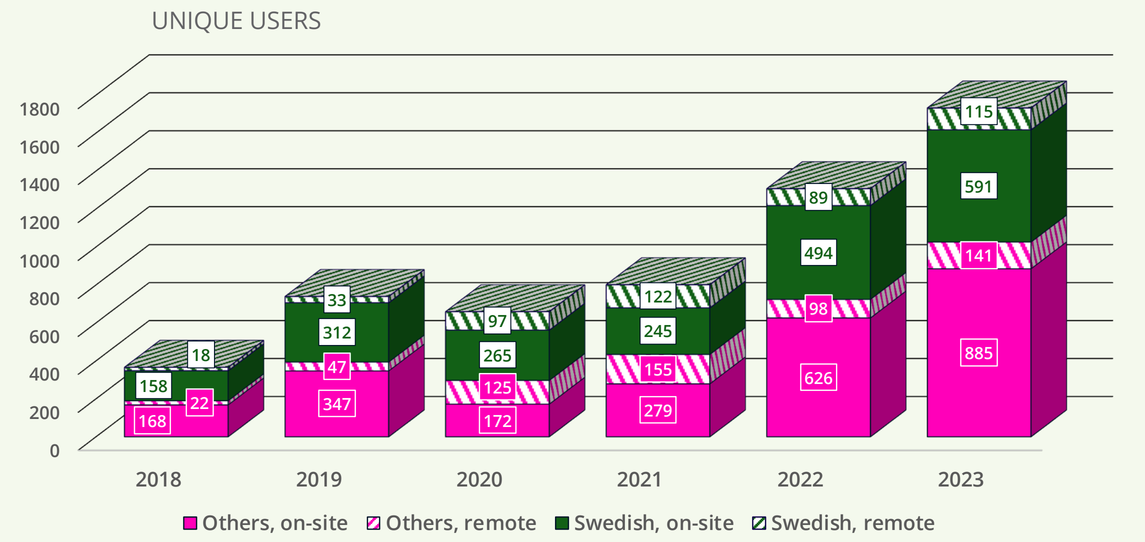


Figure 3: Unique users who visited MAX IV onsite or were granted remote access to beamlines or experiment data connected to a specific experiment, excluding MAX IV staff. Data from the pandemic years 2020–2021 is unreliable. The numbers include users whose projects were not necessarily concluded in 2023.

Development of the Swedish user community

The increase in number of unique users affiliated with Swedish home institutions has exceeded the yearly strategic goal of 10%. Since the inauguration of MAX IV in 2016, nearly 1500 researchers from Swedish institutions have used the facility at least once. MAX IV is now, by far, the most important facility for Swedish synchrotron users. There is strong evidence to suggest that MAX IV has played a crucial role in the development of the Swedish synchrotron user community.

In 2023, the total number of submitted proposals was 717, which is an increase of 14% compared to the previous year. The acceptance rate was 57%. Out of the accepted proposals, 39% were submitted by principle investigators affiliated with a Swedish home institution (see Figure 5).

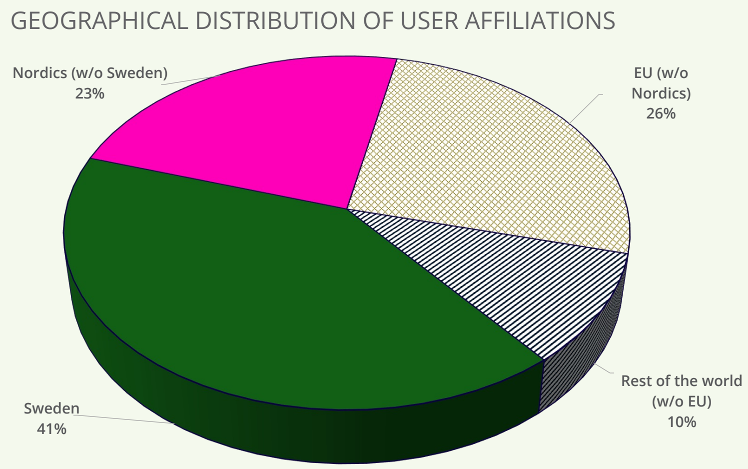


Figure 4: Geographical distribution of the home institutions of unique users in 2023, excluding MAX IV staff. The Annual Report 2022 included MAX IV staff and excluded certain remote users. Using the 2023 definition, which provides a more accurate indication, the fraction of Swedish users in 2022 was 45%.

The number of proposals submitted by Swedish principle investigators remained the same in 2023 as in 2022 (294), a stagnation that might be due to the fact that MAX IV already caters to a large part of the Swedish synchrotron community. However, their acceptance rate increased from 46% to 55%.

The demand for accessing the different beamlines varies strongly. This is largely explained by differences in operation modes, such as long experiments vs. short experiments. It is worth noting that the geographical distribution of the users' home institution affiliation also differs significantly between beamlines.

PROPOSALS ACCEPTED IN OPEN CALLS 2023 PER BEAMLINE

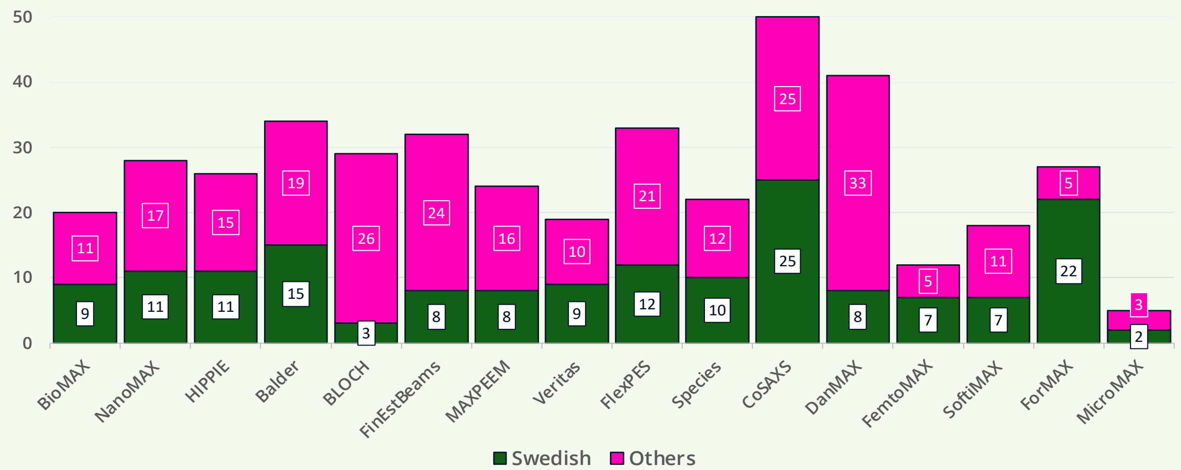


Figure 5: *Proposals accepted in Open Calls 2023 per beamline.*

BEAMLINE DEVELOPMENT

A suite of 16 funded beamlines was open for proposals for the first time in 2023. Three beamline construction projects are open at MicroMAX, DanMAX, and SoftiMAX, while three projects were completed at ForMAX, CoSAXS and NanoMAX. In addition, other beamlines are adding experimental capabilities.

New capabilities on existing beamlines

The continuous development at the beamlines led to new capabilities that were added and/or offered to external users for the first time in 2023.

Balder, the X-ray absorption and emission spectroscopy (XAS & XES) beamline for medium and hard energy X-rays, now offers external users a unique and internally developed X-ray emission spectrometer (SCANIA-2D). In addition, thanks to upgrades in the motion control system, the beamline can provide the capability to collect full EXAFS spectra in less than a second. Users have access to the secondary techniques XRD and XRF to complement XAS measurements.

BioMAX, an X-ray macromolecular crystallography beamline. Added capabilities include unattended data collection (for fragment-based drug discovery and select industrial projects) and in situ data collection of crystals in crystallisation plates.

Bloch, dedicated to high-resolution angle-resolved photoelectron spectroscopy (ARPES). The spin-ARPES station on the B-branch of the beamline became available for general proposals. Ongoing beam drift issues due to heat load on the first mirror were solved almost entirely through a combination of hardware upgrade to the chamber cooling and a new optical feedback system. The measurement manipulator on the B-branch was upgraded to 4.5 degrees of freedom with an in-house design, which has significantly helped while waiting for the 2024 procurement of a full 6-axis solution. All sample observation cameras were substantially upgraded, including the addition of a long-range microscope with <10µm resolution. Commissioning of the in situ polarimeter plus undulator 'universal mode' made substantial progress, bringing it closer to offering a unique degree of control over the beam properties at the sample in the low energy regime (<100eV).

CoSAXS, a SAXS/WAXS beamline offering a suite of complex sample environments to facilitate experiments in diverse scientific areas, including soft matter and life science. CoSAXS extended the possibility to measure the entire energy range accessible with the monochromator, 5 to 18 keV. With the WAXS detector, it is now possible to simultaneously measure in an overlapping q-range from $0.0013 < q < 2$ Å-1, depending on the sample environment at 250 Hz. The beamline added a uni-/bi-axial planar mechanical tester and an ultrasonic acoustic levitator to its sample environments.

DanMAX, a materials science beamline dedicated to in situ and operando experiments on real materials. The imaging instrument was installed, and commissioning started. This instrument allows for 3D absorption and phase contrast imaging with a spatial resolution down to 1 µm. 3D volumes can be measured as fast as one second.

FemtoMAX, the femtosecond X-ray beamline at the MAX IV short-pulse facility (SPF) tailored for ultrafast X-ray techniques. The control software for data collection was revamped with live data processing, data analysis tools, and methods. The beamline endstation for grazing incidence X-ray diffraction experiments was equipped with a cryogenic nanopositioner that counteracts sample motions under extreme environmental conditions. Beamline staff have built and tested an in-vacuum time-resolved SAXS set-up with a sample–detector distance reaching up to 6 metres.

FinEstBeAMS, a materials and atmospheric science beamline providing ultraviolet and soft X-ray radiation on two branches: one is dedicated to ultra-high vacuum studies of surfaces and interfaces, and the other branch is shared between gas-phase research and photoluminescence in solids. In 2023, continuous scanning measurements were implemented, and the solid-state endstation received several new capabilities (e.g. liquid helium cooling, an ultraviolet lamp, and thermal desorption spectroscopy).

FlexPES, offers a range of photoemission and soft X-ray absorption experiments for the surface/materials science (SMS) and low-density matter (LDM) user communities. New capabilities include: improved heat management of the M1 mirror, which allows much more stable flux intensity, absolute encoders on the sample manipulator in the SMS endstation for improved precision and reproducibility of sample positioning, enabling continuous scans of the sample surfaces for fast chemical mapping, and XPS and XAS setup for studies of liquid surfaces with flat liquid jets from microfluidic devices developed at XFEL (Hamburg). For the first time, the BL chopper and a magnetic bottle electron spectrometer were offered to external users.

HIPPIE, a beamline dedicated to ambient pressure X-ray photoelectron spectroscopy (APXPS). An advanced electrochemistry experimental platform was opened for academic and industrial users. It is available at a new branchline and allows in situ and operando APXPS for investigating batteries, corrosion, and electrocatalysis. The time-resolved APXPS capabilities were extended by the ultrafast setup, which provided microsecond time resolution with the help of piezo-driven valves and a delayline detector. Finally, a new high-temperature ambient pressure cell was commissioned and is available for user experiments requiring 1000°C under a reactive atmosphere.

MAXPEEM, is equipped with an aberration-corrected spectroscopic photoemission and low energy electron microscope (SPELEEM). The microscope underwent several upgrades, the most important involving the installation of a new, faster electron detector. The CMOS camera, an XF416 (ES), increases the framerate by a factor of ten (48 Hz) and the frame size by a factor of 4. In the reduced area (500x1000 pixels), the detector can now achieve 384 frames per second. This upgrade has significantly improved resolution, signal-to-noise ratio, and dynamic range. These enhancements are particularly crucial for the full-field microscope, enabling the study of dynamic processes on the sample surface.

NanoMAX, the hard X-ray nanoprobe at MAX IV. The new imaging endstation was completed, and the Fresnel zone plate instrument now allows for full in-vacuum operation. The endstation is available for regular user operation. The diffraction endstation received enhanced capabilities for diffraction experiments. A new Pilatus3 1M on a dedicated swivel mount allows for faster and more photon-efficient scanning X-ray diffraction experiments. A larger and gapless Eiger2 500k has replaced the Merlin detector on the robot arm. With it, more and higher quality data is possible to record for scanning X-ray diffraction and coherent Bragg diffraction experiments. Both devices are now offered for external user operation.

SoftiMAX, a soft X-ray beamline dedicated to spectromicroscopy and coherent X-ray imaging with two branch lines named STXM and CXI, respectively. The CXI branch saw first light in December 2023 and will start commissioning experiments in 2024.

SPECIES, a soft X-ray beamline with two branches: one for ambient pressure X-ray photoelectron spectroscopy (APXPS) experiments, and one for resonant inelastic X-ray scattering (RIXS) experiments. The plane grating spectrometer (PGS) was commissioned and made available for regular user operation on the RIXS endstation. The spectrometer offers high-resolution RIXS capabilities at low photon energies (approximately 25 to 120 eV). The APXPS endstation saw continuous minor improvements in both hardware and software, which makes all experiments easier for users to run and help achieve higher quality data.

Veritas, a resonant inelastic X-ray scattering (RIXS) beamline on the 3GeV ring. The closed cycle helium cryostat was further developed with new sample mounts for low temperatures (down to 9 K) and for 5-axis. The cryostat was also upgraded for freezing water and various gases to enable novel studies on molecular systems in a frozen state.

Low-Density Matter (LDM), is a cross-beamline initiative for research on gas phase molecules, liquids, aerosols, and free clusters. The molecular jet dump and correction coils of the ICE mobile endstation were upgraded, and a new aerodynamic lens sample delivery system for the generation of aerosol and nanoparticle beams had its first general user experiments. The TRISS (trapped ion spectrometer setup) was delivered and is being prepared for commissioning.

MAX IV has two main processes for orchestrating beamline developments that require internal resources. The primary process is through the Central Project Office (CPO), which coordinates all large-scale projects regarding MAX IV beamlines, infrastructure, and accelerator systems.

From the beamlines, ForMAX and MicroMAX projects have predominated CPO activities together with projects from SoftiMAX, DanMAX and FemtoMAX. Four beamline projects were initiated in 2023, which include Balder DAQ and XRD projects, M1 chamber upgrades, and new heat exchangers for beamline optical systems.

Beamline projects of smaller scale are managed through the Beamline Project Advisory Group (BPAG) process by the Beamline Office (BO). This year, 34 BPAG projects were completed, and 45 new projects were approved. These vary significantly in scope, but generally fit into three categories: emergency fixes, improvements to beamlines or equipment, and the addition of new capabilities. Examples include optics hutch water cooling improvements at DanMAX and continuous scanning at FinEstBeAMS.

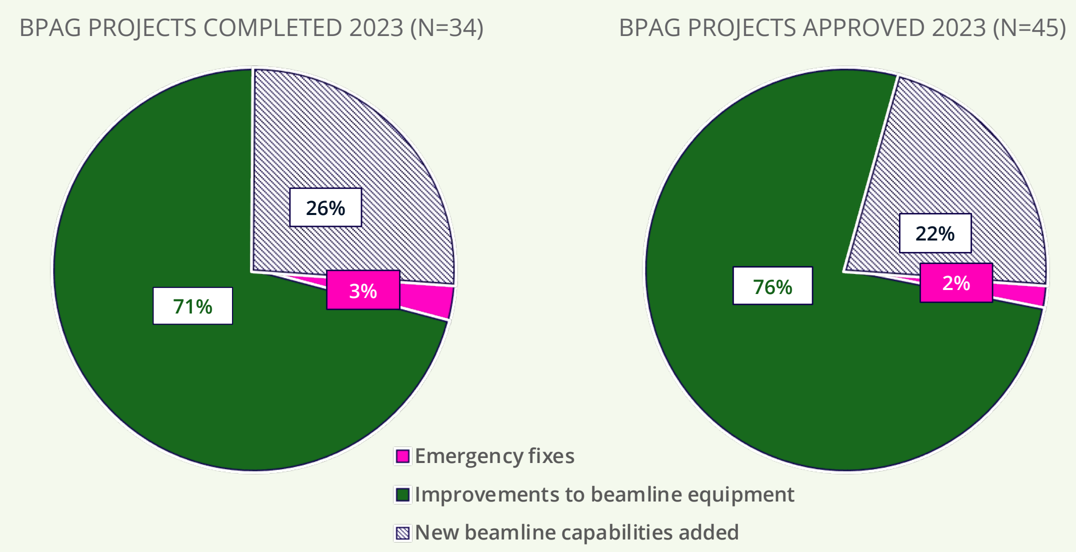


Figure 1: BPAG projects completed and approved in 2023.

APPROVED & ONGOING BPAG PROJECTS, JANUARY 2024 (N=60)

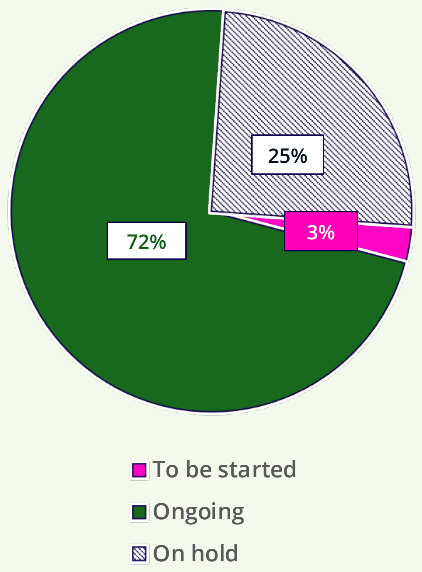


Figure 2: *As of December 2023, 60 BPAG projects were approved but not yet completed. These can be categorised as ongoing, to be started, or on hold.*

Beamline reviews

MAX IV organises periodic reviews of the beamlines to ensure adequacy and relevance of the instrumentation and scientific programs for our user communities as well as competitiveness compared to similar instruments. These beamline reviews typically occur every three to five years and aim to assess scientific productivity and associated medium and long-term technical and strategic development plans. In 2023, the activities of MAXPEEM and Balder beamlines were evaluated in separate reviews, while BioMAX and MicroMAX beamlines were reviewed jointly as they operate very closely together. The review outcomes were presented and discussed with our Science Advisory Committee (SAC).

New beamlines

Beginning in summer 2023, The Wallenberg Initiative Materials Science for Sustainability (WISE) awarded MAX IV funding for the development of three conceptual design reports (CDRs) for new beamlines. The reports were based on previously submitted Expressions of Interest (EoIs).

Three CDRs were submitted to WISE for evaluation at the end of 2023 through a collaboration between MAX IV and the potential user community of each EoI.

- A Spectroscopy Beamline Supporting Materials Science for Sustainability
- An Imaging Beamline Supporting Materials Science for Sustainability
- A Diffraction Beamline Supporting Materials Science for Sustainability

INDUSTRY UTILISATION AND ENGAGEMENT

As a crucial tool for advanced research on materials and processes, MAX IV continues to experience a steady increase in industrial utilisation, supporting businesses in the transition to sustainable materials and manufacturing.

Increasing industrial use

In 2023, 14% of MAX IV beamtime was utilised by the industry. It was accessed either through collaborative open access or proprietary access (Figure 1). Proprietary industrial use has grown significantly since 2018, reaching 834 hours in 2023. This increase is almost entirely attributed to protein crystallography performed at BioMAX beamline. Most notably, FragMAX, a user facility for crystallographic fragment screening, attracted three new proprietary user groups in 2023, accounting for a large amount of beamtime. Additionally, 29 hours of proprietary access to the optics lab were sold.

As synchrotrons worldwide upgrade to 4th generation and enter so-called dark periods, companies look for alternative suppliers of protein crystallography services. With more shutdowns anticipated in the coming years, MAX IV strives to use this opportunity to reach new companies and remain a competitive facility for macromolecular crystallography (MX) services.

There is a small decrease in collaborative industry use through open access which is thought to be connected to the two-year cycles of the BAG proposals for protein crystallography. On the positive side, MAX IV has received an increased number of industry-connected projects related to battery research and energy materials.

BEAMTIME HOURS EXTERNALLY USED IN 2023 BY TYPE OF ACCESS

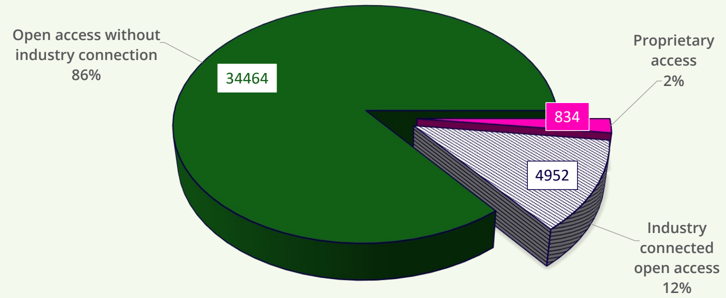


Figure 1: *No. of beamtime hours externally used at MAX IV in 2023 divided by type of access.*

Access support for industry

External funding, primarily through initiatives such as industrial pilot projects funded by Vinnova, has proven to temporarily boost the proprietary use of synchrotrons. Between 2018 and 2023, Vinnova allocated substantial funds to promote industrial utilisation of synchrotrons and neutron sources, in turn influencing MAX IV's user statistics. While these pilot projects successfully expanded proprietary use beyond the pharmaceutical industry, the 2023 data underscores the noticeable gap in funding in 2022 (Figure 2). It highlights a key observation: relying on support-funding does not suffice to prompt companies to adopt the advanced techniques independently.

PROPRIETARY BEAMTIME HOURS SOLD 2018-2023

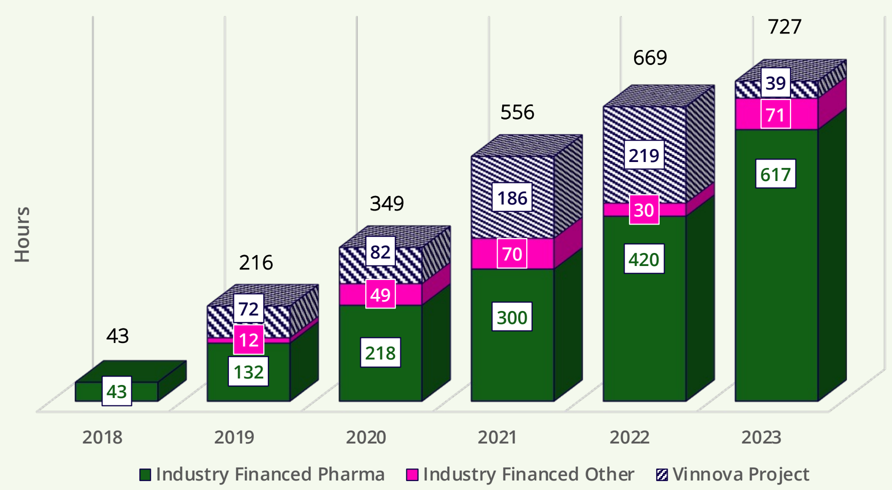


Figure 2: *No. of proprietary beamtime hours sold over the past six years (1 Jan-31 Dec), indicating hours of beamtime funded through Vinnova pilot projects and purely industry-funded beamtime.*

The pilot projects had a clear impact, rendering over 100 industry case experiments conducted at synchrotrons and neutron sources. Some are published as industry cases on the MAXESS website, providing a basis for further discussion. However, the funding landscape needs broader opportunities to innovate by creating new services or sample environments, paving the way for new industrial user communities. For instance, the Swedish Research Council's grant "Tillgängliggörande av Infrastruktur" was pivotal in establishing the FragMAX platform and currently supports the InfraLife project.

Broadening the industrial userbase

Ensuring long-term integration of synchrotron techniques within the industry requires long-term efforts, such as establishing platforms for collaboration between industry and synchrotrons in specific research areas. In 2023, MAX IV's continued its collaboration with Alfa Laval, targeting the metals and engineering sector. It included a two-day workshop with MetalBeams at MAX IV with support from Jernkontoret, where eight companies experienced a hands-on corrosion assessment experiment at HIPPIE beamline conducted by researchers from MAX IV, Lund University, and Swerim. MAX IV also organised meetings with companies in the mining and battery sectors. Within InfraLife, MAX IV organised a visit for SciLifeLab to MAX IV and ESS to highlight life science capabilities and foster connections among scientists and directors. MAX IV's imaging beamline experts contributed to InfraLife's webinar series on imaging capabilities.

An incubator-based methodology for reaching potential industry users was established in the project "MAXESS SmiLe: SMEs to LSRI". The project, involving 12 companies, concluded in 2023 and resulted in three experiments at large-scale research infrastructures. The MAXESS website was further developed, and project members are discussing ways to build upon the MAXESS achievements.

In certain industry sectors, the knowledge level of MAX IV and its techniques is so advanced that integrating it into the value chain is a matter of time and practicality. In 2023, over 20 identified advanced R&D groups were invited to in-depth discussions at MAX IV about practical questions such as sample environments. Several of the groups have the potential to become MAX IV users in the next few years.

Employing a collaborative approach

EU projects and consortia offer valuable opportunities to support industry in accessing MAX IV. For instance, MAX IV provides supported industry access to two beamlines through the project ReMade@ARI focusing on circular economy materials research. In 2023, MAX IV contributed to establishing a network of procurement officers from the ten member organisations of the LEAPS consortium (League of European Accelerator-based Photon Sources). The aim is to exchange best practices, support SME suppliers, and expand the supplier base to reduce costs and secure access to the highest quality suppliers.

In May 2023, MAX IV hosted a three-day workshop for peers within the EU-funded LEAPS-INNOV project. It brought together 29 representatives from industrial liaison offices at 17 light sources who discussed critical efforts to enhance the industry's use of light sources. MAX IV also hosted visits by HALRIC (the Hanseatic Life Science Research Infrastructure Consortium), dedicated to fostering cross-collaboration among its 20 partners and the industry through pilot project funding. Additionally, MAX IV participates in the HALRIC project's review committee to promote industrial use.

SCIENCE AT MAX IV

FOREWORD

In 2023, scientific productivity reached a record high with over 50% increase in the number of publications from MAX IV compared to the previous year.

It was a year of remarkable progress and success – a testament to the collective effort of MAX IV's staff and its growing user communities. Not only were the instruments and endstations further developed, but the beamline portfolio now includes 16 beamlines that support the User Science programme and advanced science.

Many of the science examples in this chapter are important puzzle pieces that contribute to a better, sustainable future and support the development of new and emerging technologies. Examples include the optimisation of catalysts for cleaner air production and the generation of sustainable fuels, energy materials that support the generation and storage of non-fossil fuels, and contributions to a better understanding of cancer radiotherapy.
It is also important to note that about one-fifth of the user research conducted at MAX IV is connected to industry. One example highlighting this is the study on carbon-based particle filters.

The science is the result of MAX IV's staff and the user communities' dedication, motivation, and engagment in contributing to a compelling Science programme. For that, MAX IV is very grateful. The hope is to inspire further use of MAX IV for future research needs.

The MAX IV publication database contained 226 peer-reviewed articles in 2023, an increase of 44% compared to 157 publications in 2022.

The total number of publications (see Figure 1, dashed line) consists of journal articles discussing data measured at MAX-Lab (pink) and at MAX IV (green). Publications that discuss data measured both at MAX-Lab and MAX IV are designated as MAX IV. Articles from MAX IV staff that do not involve MAX IV data, e.g., theoretical or technical work and measurements performed at other facilities, are counted as MAX IV publications. A detailed breakdown is provided (Figure 3). Publication details are also available on the MAX IV website at publications.maxiv.lu.se.

Many years after the closure of MAX-Lab and the inauguration of MAX IV in 2016, the number of journal articles based on data acquired at MAX-Lab continues to decrease, i.e., five articles in 2022. It represents 2% of the total number of publications (Figure 1). This number is expected to continue to decrease.

The decrease in articles based on MAX-Lab data is compensated by a large and sustained growth in the number of publications based on MAX IV data (green), which increased by 51% in 2023, as indicated by the arrow in Figure 1. This reflects the growing scientific output of the laboratory and is consistent with the increasing number of beamlines that has transitioned to User Operation (e.g. 16 beamlines by December 2023) and the increased capabilities of each beamline. The trend is expected to continue in 2024.

The cumulative number of MAX IV publications since 2016 increased to 651 publications in 2023, a 51% increase compared to 2022. 10 PhD and 11 MSc and BSc theses were completed in 2023 using results obtained at MAX IV.

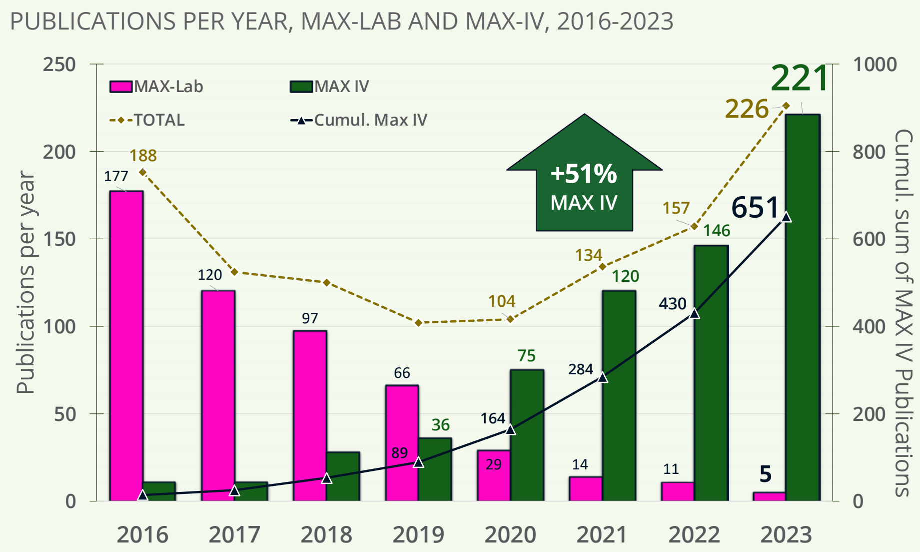


Figure 1: Number of publications per year based on data measured at MAX-Lab (pink) and MAX IV (green). The dashed line indicates the total number of publications per year (MAX IV and MAX-Lab). The solid line displays the cumulative number of MAX IV-only publications since 2016.

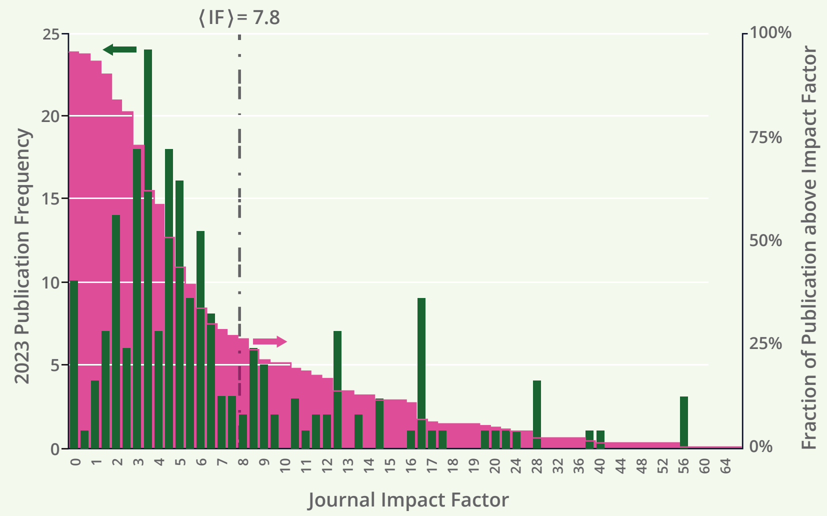


Figure 2: Histogram (left axis): 2023 Publications frequency as a function of the 2023 published journals impact factor (IF). Solid line (right axis): Fraction of 2023 publications above a specific journal impact factor IF. The dash-dotted line indicates the average impact factor <IF> = 7.8.

A graphical representation of MAX IV's scientific impact of the work performed at MAX IV is presented in Figure 2. It displays the histogram (green) of the 2023 publications frequency as a function of the most recent journal impact factor (2023 Journal Citation Report from Clarivate and using the two-year average impact factors when available). An impact factor of zero (0) is allocated to those publications that cannot be associated with an impact factor.

The following can be noted:

- The average impact factor of all publications in 2023 is <IF> = 7.8.
- The average impact factor remains large and equivalent to <IF> = 7.8 for 2022.
- About 27% of 2023 publications are in journals with an impact factor larger than the average impact factor <IF>. This is consistent with the statistics from 2022 publications.
- This indicates that the 51% increase in publications in 2023 remains of high quality compared to previous years.
- Five publications are in journals with an impact factor above 30: Science (3), Nature Materials (1), and Signal Transduction and Targeted Therapy (1).
- Ten publications are indicated with an Impact factor of zero (0) because no impact factor is currently available. They were discarded from the calculation of the average impact factor.

Figure 3 presents the distribution of 2023 peer-reviewed publications related to data acquired before 2016 at MAX Lab (striped-blue), with any MAX IV beamlines (green), and the ones associated with the development of our accelerator complex (yellow). Publications connected to data acquired both at MAX-Lab and MAX IV are credited to the respective MAX IV beamline. Beamlines are ordered vertically from top to bottom according to when they were introduced to User Operation.

The following can be noted:

- BioMAX beamline contributed to 24% of the 226 publications for 2023.
- The scientific productivity of the first beamlines (NanoMAX, HIPPIE, FinEstBeAMS, BLOCH, and FlexPES) continued to increase. All exceed the threshold of 9 publications per beamline.
- A leap in science productivity from Balder beamline from 7.5 articles in 2023 to 21 in 2023, an increase of 180%.
- Veritas beamline has addressed continuous technical challenges over the past few years. Expert commissioning users and regular users performed experiments in 2023, and the User Science programme is expected to ramp up as the technical performance of the RIXS instrument matures.

- The science productivity from FemtoMAX beamline remained low and of concern. The beamline team is addressing this, and publications are foreseen to come out in 2024. FemtoMAX will be evaluated within the framework of the periodic beamline reviews in mid-2024.
- SoftiMAX, ForMAX and DanMAX beamlines entered User Operation in 2022. The scientific productivity of these beamlines is expected to grow rapidly over the coming years. There is already a steep increase in productivity for DanMAX from 5 to 18 publications between 2022 and 2023.
- Publications are not yet expected from MicroMAX beamline as it only accepted expert user experiments in December 2023.
- 21 publications do not discuss data acquired at MAX IV (nor MAX-Lab) but have MAX IV staff as co-authors. These staff are usually involved with technical or engineering work, but also measurements and studies performed at other facilities. These papers represent 10% of the total number of publications in 2023.

PUBLICATIONS 2023 PER SOURCE OF THE DISCUSSED DATA

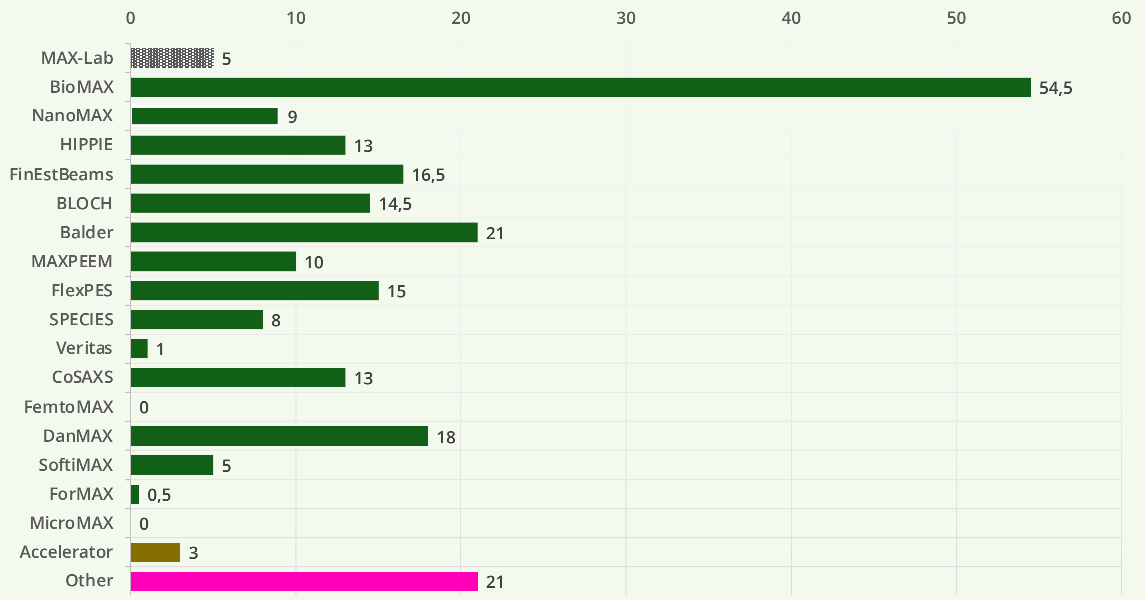
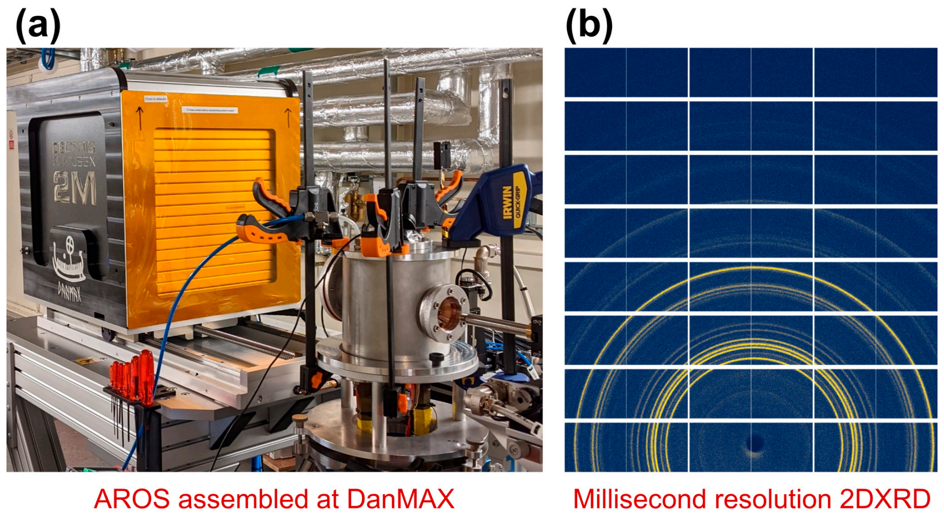


Figure 3: Number of publications in 2023 discussing data from MAX-Lab (striped-blue) or the MAX IV beamlines (green). Publications related to both MAX IV and MAX-Lab measurements are credited to the respective MAX IV beamline. Beamlines are ordered according to when they were introduced in our User Science programme, from top to bottom. Publications based on data acquired at more than one instrument are prorated to the number of beamlines involved. Accelerator: Number of publications related to the MAX IV Accelerator Division. Other: Number of publications from MAX IV staff unrelated to a measurement performed at our beamlines (e.g., engineering or theory article, collaboration with other facilities, etc.)

Following through: in situ observation of synthesis–structure–property dynamics in magnets

DanMAX

Magnetic materials are vital components of the green transition since they are at the heart of electromotors for electric vehicles and generators in wind turbines, among others. Magnetic Matter Aarhus research group used a high-energy two-dimensional synchrotron X-ray diffraction (2D-XRD) at DanMAX beamline combined with the Aarhus Rapid Ohmic Sintering (AROS) setup to look closely into in situ sintering of magnetic ceramic $SrFe_{12}O_{19}$.



AROS set-up at BioMAX and a representative 2D diffraction image of the $SrFe_{12}O_{19}$ sample obtained by the detector during the in situ experiment with 4 ms time resolution.
Credit: *Priyank Shyam (research team).*

Utilising the brilliant X-rays and the AROS setup, researchers could investigate seven orders of magnitude in length scale from atomic scale (Å), nanoscale (10-100 nm) to information about the orientation of crystallites on the micrometer scale with a time resolution of only 4 ms.

The study proves that the technique can provide a valuable understanding of the chemical process during sintering and texture evolution to improve the synthesis procedure and to design better materials for future magnets, thermoelectric, piezoelectric, and energy storage.

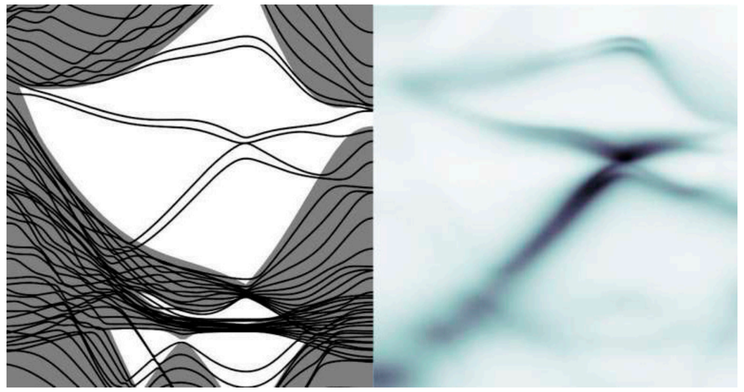
Publication
P. Shyam, et al. Sintering in seconds, elucidated by millisecond in situ diffraction.
Materials Today 35, 101960 (2023).
DOI: 10.1016/j.apmt.2023.101960

Long-awaited technique for growing monolayer honeycomb SiC discovered at MAX IV

Bloch

The "wonder material" graphene has an enormous presence in contemporary physics research. At the periphery, researchers continued to be curios about 'graphene-like' allotropes that swap out one or both of the carbon atoms to bring new and desirable properties, e.g.; the long-theorised allotropes based on silicon carbide (SiC). SiC should introduce a large electronic bandgap, an attractive property for new electronic or opto-electronic devices. Unfortunately, these allotropes are much trickier to create in the laboratory than graphene, and SiC has been a noteworthy holdout.

However, an unexpected turn in a graphene study at the Bloch beamline has led to the first realisation of large-area monolayer honeycomb SiC. Putting to work angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations, researchers from MAX IV, Lund University, Chalmers University of Technology, and Linköping University were able to conduct a bottom-up synthesis of monocrystalline, epitaxial monolayer honeycomb SiC atop ultrathin transition metal carbide films on SiC substrates.



Calculated and measured band structure of SiC.
Credit: *Craig Polley.*

The technique involves introducing both silicon and carbon atoms to the surface of a tantalum- or niobium-carbide crystal. In their study, this was achieved by annealing metal carbide films in just the right conditions to make the underlying SiC substrate start to decompose. The Si and C atoms migrate to the surface and form single crystal honeycomb SiC. In this 2D state, the large-area, high-quality SiC was stable in vacuum at high temperatures, up to 1200 °C.

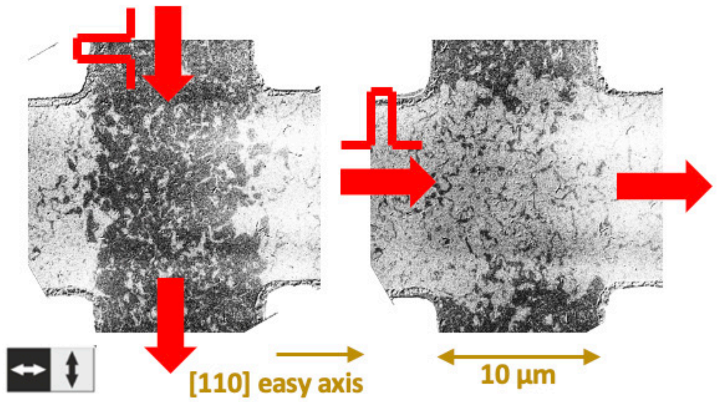
This breakthrough has established a new research direction to begin further exploration of the growth and characterisation of honeycomb SiC, eventually perhaps leading to novel technological applications.

Publication
C. M. Polley et al. Bottom-Up Growth of Monolayer Honeycomb SiC.
Physical Review Letters 130, 076203 (2023).
DOI: 10.1103/PhysRevLett.130.076203

A promise realised for memory storage with antiferromagnetic spintronics

MAXPEEM

In the realm of device memory applications with spintronics, antiferromagnets are a promising advancement to achieve significantly faster writing speeds (Terahertz range). The alternating alignment of their microscopic magnetic moments creates zero net magnetisation.



Orientation of the Néel vector of Mn_2Au(001) thin films after sending current pulses with different length and direction (yellow arrows) through a patterned cross structure oriented parallel to the easy [110] directions.

Research led by Johannes Gutenberg University Mainz in Germany explored the so-called current pulse driven Néel vector rotation, performing a current pulse induced manipulation of the orientation of the axis along which the alternating magnetic moments of the antiferromagnet Mn_2Au (manganese-gold compound) are aligned. The orientation is a critical detail used to encode information in antiferromagnet memory devices. The Néel vector of Mn_2Au was reoriented reversibly in the complete area of cross-shaped device structures.

Imaging the orientation of the alignment axes of the magnetic moments in Mn_2Au thin film samples was done with photo-electron emission microscopy (PEEM) at MAX IV's MAXPEEM beamline. The results demonstrate the possibility to write long term stable information by single current pulses into macroscopic areas of device structures.

The work enhances knowledge for the application of non-volatile Magnetic Random-Access Memory (MRAM) to replace the volatile Random-Access Memory (SRAM/DRAM) of current computers, and therefore greatly reduce their power consumption.

Publication

S. Reimers et al. Current-driven writing process in antiferromagnetic Mn2Au for memory applications.

NATURE COMMUNICATIONS 14, 1861 (2023).

DOI: 10.1038/s41467-023-37569-8

Deepening knowledge of low-k materials with photoluminescence

FinEstBeAMS

An international research group investigated the optically active defects in ultraviolet-induced photoluminescence of organosilica films to understand their origin and nature. The researchers used three types of organosilica glasses including, periodic mesoporous organosilica with ethylene and benzene bridges, a film with a hyperconnected structure of benzene bridges, and a film with a classic low-k (low-dielectric) structure of methyl groups and random porosity.

Their results revealed that luminescence sources are not associated with the presence of oxygen-deficient centres, and that the luminescence sources are the carbon-containing components part of the low-k-matrix as well as the carbon residues formed upon removal of the template and UV-induced destruction of organosilica samples. Photoluminescence intensity was observed to increase with porosity and internal surface area. Luminescence and luminescence excitation spectra were measured with the photoluminescence endstation at MAX IV's FinEstBeAMS beamline.

Porous organosilica films have many exciting applications such as catalysis, drug and gene delivery to microelectronics and ultra-large-scale integration (ULSI) technology where millions of transistors are integrated or embedded on a single silicon semiconductor microchip.

Abstract depiction of photoluminescence.

Publication

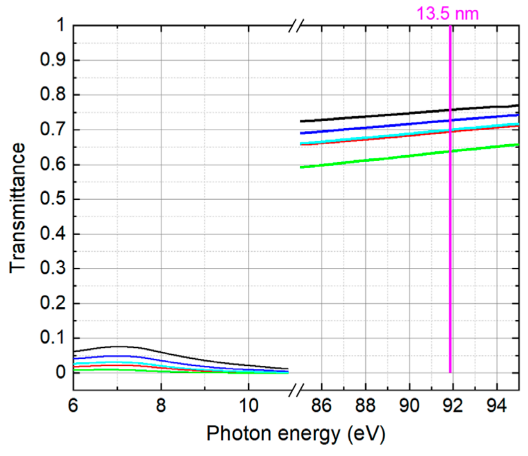
M. Rasadujjaman et al. UV-Excited Luminescence in Porous Organosilica Films with Various Organic Components.

NANOMATERIALS 13, 1419 (2023).

DOI: 10.3390/nano13081419

Fine-tuning the next-generation debris filter for industry made from carbon nanotubes

FinEstBeAMS



Filtering properties of different types of filter designs.

In the semiconductor manufacturing process, a filter is needed to prevent particles and ions from contaminating the silicon wafer and block out undesired wavelengths of light. Finnish carbon nanomaterial development company Canatu Oy develops and tailors such filters in the shape of carbon nanotube membranes for different industrial uses. The membranes should transmit the light used for the lithography process in the EUV range while blocking the 100-200 nm wavelength.

Canatu collaborated with the research team at MAX IV beamline FinEstBeAMS to do precise transmission measurements in both DUV and EUV optical ranges with precisely controlled parameters.

FinEstBeAM's coverage of the entire energy range from 4.5 eV (276 nm wavelength) to well above the EUV range at 92 eV (13.5 nm) offered a unique possibility for testing and optimising the material's properties.

"We highly value the availability, fast turnaround, and the reliability of results in our collaboration with Max IV Laboratory," says Emile van Veldhoven, Senior Development Engineer, Canatu.

ADVANCED MATERIALS

Unusual electron pairing gives clue to high-temperature superconductivity

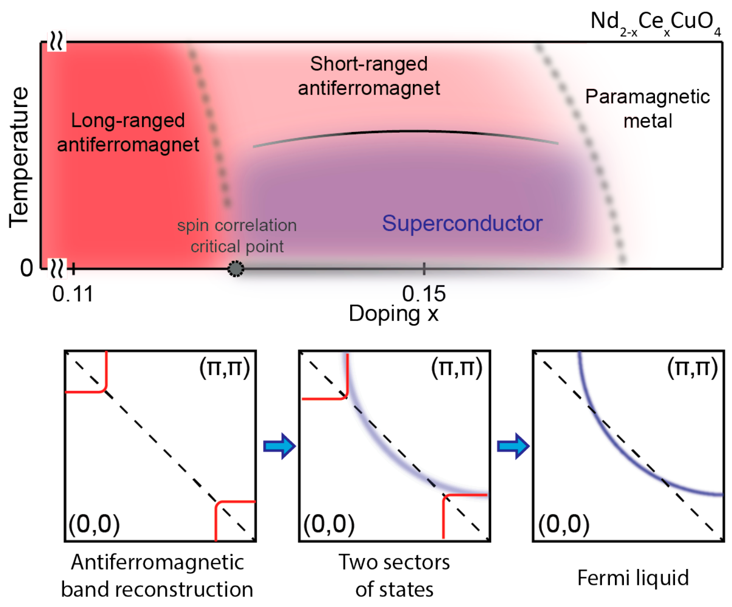
Bloch

A team of researchers have studied the antiferromagnetic electron-doped high-temperature superconducting material $Nd_{1.85}Ce_{0.15}CuO_4$. Cuprates are well-known model systems with strongly interacting electrons and they exhibit several unusual phenomena, including unconventional superconductivity.

For $Nd_{1.85}Ce_{0.15}CuO_4$ and other similar materials, the electrons within the same band seem to both provide the glueing force and themselves get glued together to give rise to superconductivity, giving rise to a longstanding dilemma dating back more than three decades. The antiferromagnetic properties of $Nd_{1.85}Ce_{0.15}CuO_4$ are the key to superconductivity.

The research results show that the low energy band for electrons is split into two components. One of these components forms the expected antiferromagnetic band.

Surprisingly, another gossamer – meaning very faint – band was also found, and it turns out that the gossamer states form because the magnetic properties of the atoms fluctuate. Now, the electrons can exist in two states, one that can give rise to the glueing interaction and one that can host the electrons being glued together. The results have implications for further development of high-temperature superconductors.



Properties of $Nd_{1.85}Ce_{0.15}CuO_4$ as a function of temperature and doping.

Publication

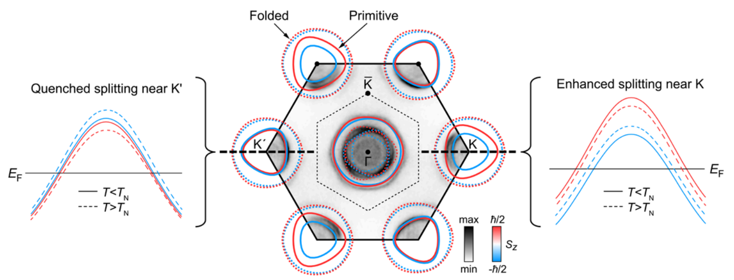
K-. J. Xu et al. Bogoliubov quasiparticle on the gossamer Fermi surface in electron-doped cuprates.
Nature Physics 19, 1834 (2023).
DOI: 10.1038/s41567-023-02209-x

High-resolution surface studies important step for valleytronics

Bloch

In most of today's electronics, the electron charge is the key to storing and handling information. To improve the efficiency of future devices, alternative technologies are being researched to develop next-generation devices which exploit additional electronic degrees of freedom to store and process information. In valleytronics, extrema in the momentum space of the band structure, referred to as 'valleys', are exploited.

Monolayer transition metal dichalcogenides offer hope for functioning valleytronic devices, owing to the presence of degenerate, but inequivalent, valleys with distinct spin textures (so-called spin-valley locking), which opens the potential to access and harness a valley pseudospin. However, it has remained challenging to control the valley-spin splittings, with attempts to achieve this, for example by applying magnetic fields, leading to only modest changes of a few millielectronvolts.



Calculation overlaid with ARPES data from intercalated transition metal dichalcogenide $V_{1/3}NbS_2$.

In the present study, the researchers used the small intense MAX IV beam to study the micrometre sized magnetic domains of the metal intercalated transition metal dichalcogenide $V_{1/3}NbS_2$ through its magnetic transition temperature. The interplay between relativistic effects of electron motion and magnetism at the surface results in the largest control over valley-spin splittings observed to date.

Publication

B. Edwards et al. Giant valley-Zeeman coupling in the surface layer of an intercalated transition metal dichalcogenide.

Nature Materials 22, 459 (2023).

DOI: 10.1038/s41563-022-01459-z

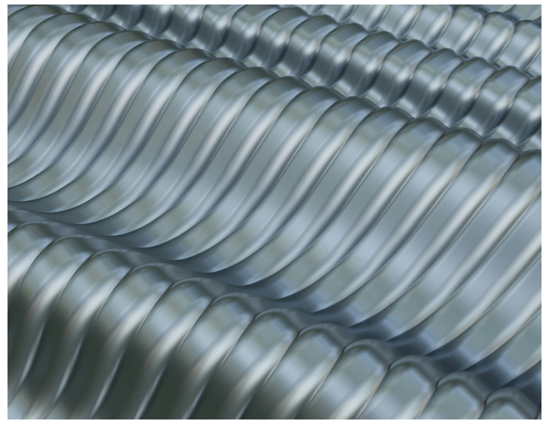
Elusive corrosion process unveiled by multimodal X-ray investigation

HIPPIE

Corrosion is a big economic and safety issue for all kinds of metal constructions. A metal material may be naturally corrosion-protected by its' own oxide (passive film) forming on the surface, like stainless steel. Environments may sometimes be too harsh for stainless steel to maintain the protective layer. In such cases, Ni-based alloys are a popular alternative.

In the present study, researchers investigated a Ni-Cr-Mo alloy to understand what really happens when it gets corroded. Protective oxide films at a solid-liquid interface are far from trivial to study. The researchers combined several X-ray techniques in a multimodal approach to analyse the thickness, composition, and chemical state of the oxide film, the changes of the underlying metal, and metal elements dissolved into the corrosive liquid.

The researchers conclude that the passivity breakdown of the Ni-Cr-Mo alloy is correlated with the oxygen evaluation process of the aqueous electrolyte. The surface gets enriched in molybdenum oxides and acts as a catalyst facilitating the oxygen evolution, coupled with nickel and chromium dissolution from the material. This is a different process than other traditional corrosion processes and must be taken into account when working with materials that are catalytically active in this way.



The researchers concluded that the passivity breakdown of the Ni-Cr-Mo alloy was correlated with the oxygen evaluation process of the aqueous electrolyte.

Publication

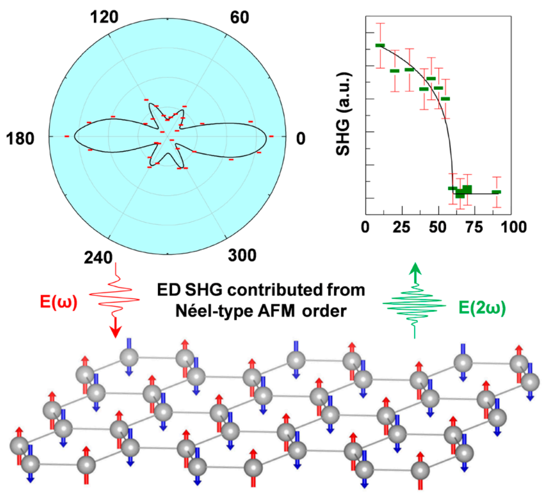
A. Larsson et al. The Oxygen Evolution Reaction Drives Passivity Breakdown for Ni–Cr–Mo Alloys.

Advanced Materials 35, 2304621 (2023).

DOI: 10.1002/adma.202304621

Way forward for studying 2D antiferromagnets opens for applications

MAXPEEM



Polarisation resolved second harmonic generation (SHG) and SHG as a function of temperature on a Néel-type antiferromagnet.

A research team has recently found an effective way of probing two-dimensional antiferromagnets. They investigated the magnetic configuration and spin-correlation coupling effects of VPS_3 through optical routes. Moreover, an interlayer exciton–magnon coupling is observed in the two-dimensional heterointerface of monolayer semiconductor WSe_2 – few-layer antiferromagntic insulator VPS_3. The result opens up for further investigations on using two-dimensional antiferromagnets for opto-spintronics or antiferromagnet-based quantum information technologies.

Two-dimensional antiferromagnets were just recently discovered and seem to be promising materials for information storage devices. They have been challenging to study because they do not have a net magnetic moment. The difficulties of detecting the antiferromagnetic order and manipulating the correlated magnetic coupling behaviour has been a seemingly insurmountable barrier, limiting their further applications.

The researchers studied a material called VPS_3 by combining several methods. VPS_3 exhibits a rare Néel-type antiferromagnetic structure, which means breaking both spatial-inversion and time-reversal symmetries. The material is challenging to synthesize and has therefore up to this point remained relatively uninvestigated.

Publication

C. Liu et al. Probing the Néel-Type Antiferromagnetic Order and Coherent Magnon–Exciton Coupling in Van Der Waals VPS3.

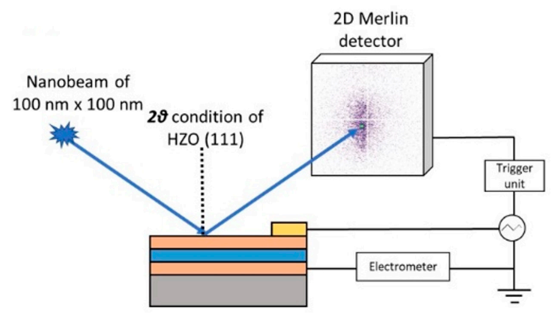
Advanced Materials 35, 2300247 (2023).

DOI: 10.1002/adma.202300247

Understanding hafnia ferroelectricity paves the way for low power electronics

NanoMAX

Ferroelectricity in hafnia has gained traction both technologically and scientifically since its discovery in 2011. The discovery has pushed the area of low power ferroelectric electronics into the scientific spotlight. The origins of the ferroelectricity in hafnia is different from that of conventional ferroelectrics.



Setup of the experiment.

In this recent study the features of unconventional ferroelectricity in rhombohedral and epitaxial hafnia zirconate thin films are investigated. The key result is that the piezoelectric nature related to the crystallographic polar axis is decoupled from ferroelectric switching.

The research team has investigated the role of oxygen vacancies in ferroelectric switching in an earlier study. Then there was doubt given that the experiments performed in the earlier study were in real time, and not really at the switching timescales of hafnia. In the present study they addressed this issue, by following the tiny piezoelectric behavior of hafnia when it is ferroelectrically switching.

The result provides useful guidelines for materials design to address current problems of endurance in ferroelectric hafnia and to design unconventional ferroelectrics similar to hafnia that are silicon compatible.

Publication

E. Stylianidis et al. Investigating the Electromechanical Behavior of Unconventionally Ferroelectric Hf0.5Zr0.5O2-Based Capacitors Through Operando Nanobeam X-Ray Diffraction.

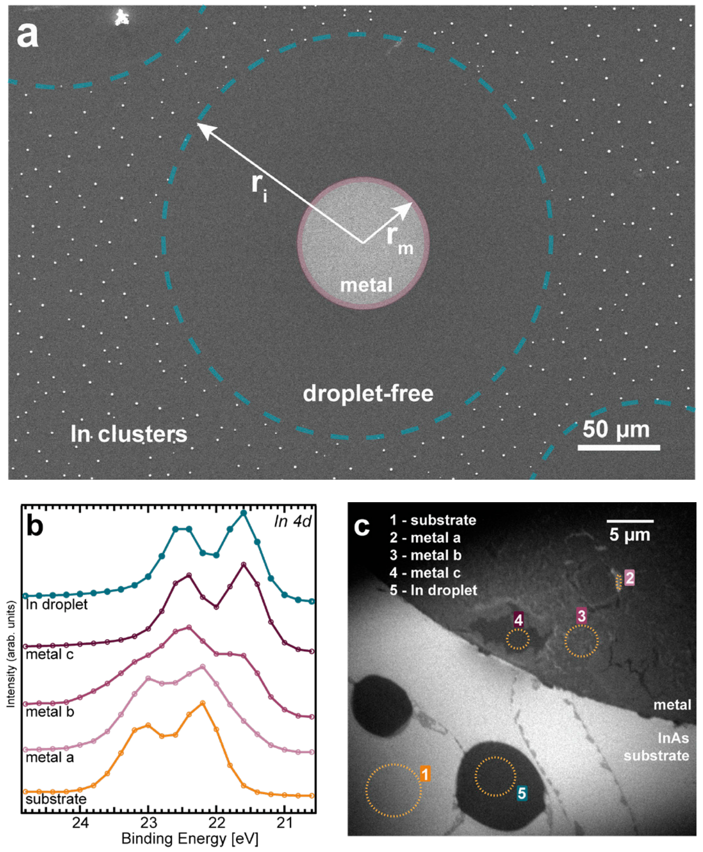
Advanced Electronic Materials 9, 2201298 (2023).

DOI: 10.1002/aelm.202201298

ADVANCED MATERIALS

Eliminating droplets: A novel approach for advanced semiconductor design

MAXPEEM



(a) SEM image of the distinctive droplet-free zone around the metal pattern after heating the sample to 600°C. (b) XPEEM data set of the In4d core level taken at the positions indicated in (c). It is evident that In atoms diffuse into the metal stack and create a variety of different chemical environments by bonding with Pd, As or itself.

The formation of droplets on the surface of compound semiconductors is a common limitation to its temperature range during device manufacturing, restricting the synthesis of planar devices to lower temperatures.

To propose a solution to this, researchers from NanoLund used surface-sensitive measurement methods, including photoelectron microscopy measurements at MaxPEEM beamline, on InAs surfaces displaying metal stacks with 5 nm Al topped by 20 nm Pd, commonly used as contact materials on compound semiconductors. The experiment shows that lithographically defined Al/Pd metal stacks on an InAs wafer surface can enable droplet-free areas adjacent to the metal stack for temperatures up to 600°C in an average UHV system. The excess In atoms on the InAs surface diffuses into the metal, forming various chemical environments. The novel method can locally tune the formation of nano and micron-sized droplets near the metal, significantly increase the temperature window where no droplets will develop on the semiconductor surface and easily be adapted for other compound semiconductors systems, like GaAs, InP or InSb.

In the long run, this result will be relevant for designing and manufacturing quantum computers, optoelectronics, and various neuromorphic applications where exploring different synthesis temperature regimes can enable new advanced systems.

Publication

S. Benter, et al. Geometric control of diffusing elements on InAs semiconductor surfaces via metal contacts.

Nature Communications 14, 4541 (2023).

DOI: 10.1038/s41467-023-40157-5

ADVANCED MATERIALS

Investigating future metal halide perovskites applications

NanoMAX

With the continuous development of metal halide perovskites (MHP) into applications such as solar cells, light-emitting diodes and X-ray detectors, more fundamental knowledge is required for future technological designs. A key component of many such devices is heterostructures, where two materials with different bandgaps are combined in the same crystal.

A team from Synchrotron Radiation Research and NanoLund, Lund University, used nanofocused scanning X-ray diffraction (XRD) and X-ray fluorescence (XRF) with a 60 nm beam to image and quantify composition, strain, and ferroelastic domains within axially heterostructured MHP $CsPbBr_3$–CsPb(Br(1−x)Clx)3 nanowires. $CsPbBr_3$ is an MHP that emits green light, with possible applications in light-emitting diodes and X-ray scintillators. Ferroelastic domains of different types were observed in both the heterostructured and reference nanowires.

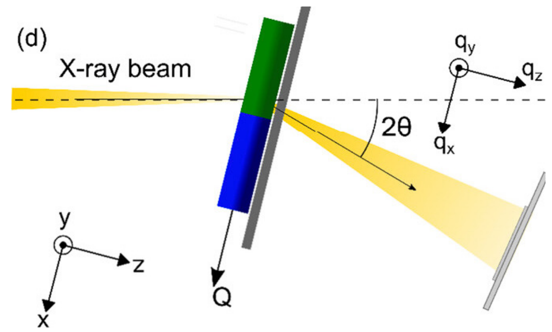


Illustration of the nano-XRD experimental setup at NanoMAX. Image taken from the publication.

Scientists also observed undesired diffusion of Cl, which is a challenge for optoelectronic devices based on MHP heterostructures since it reduces control of the bandgap. It was not possible to gather this information with lower-resolution methods.

The results show that an X-ray nanobeam like MAX IV's NanoMAX can be used to image the strain and composition within single perovskites nanowire heterostructures to better inform the design of future electronics.

Publication

S. Hammarberg et al. Nanoscale X-ray Imaging of Composition and Ferroelastic Domains in Heterostructured Perovskite Nanowires: Implications for Optoelectronic Devices.

ACS Applied Nano Materials 6, 17698 (2023).

DOI: 10.1021/acsanm.3c02978

ADVANCED MATERIALS

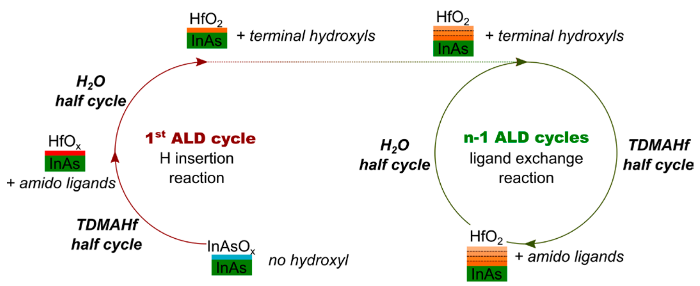
Employing APX-PS to ALD, a new outlook into semiconductor surface reactions

HIPPIE

Researchers from Synchrotron Radiation Research, Lund University, had a mission to improve interfaces in III-V semiconductor-based devices by looking into the atomic layer deposition (ALD) of the high-k oxide HfO_2 on InAs and challenging the traditional ligand exchange mechanism.

Employing in situ and operando ambient pressure X-ray Photoelectron Spectroscopy (AP-XPS) studies at HIPPIE beamline, the experiment showed a successful self-cleaning process during the first ALD half-cycle upon an unexpected reaction pathway and the efficient formation of a uniform HfO_2 layer during the second half-cycle.

These results challenged the established ligand exchange mechanism of ALD reactions, a crucial insight into improving the interface quality of the $InAs/HfO_2$ stack.



Schematic illustration of the experiment. Credit: Giulio D'Acunto.

These advancements promise transistor application with ultra-high switching frequencies coupled with reduced power consumption, marking a potential advancement beyond the capabilities of current silicon-based electronics.

By employing in situ AP-XPS for the first time, scientists obtain new insights into the active surface chemistry during HfO_2 deposition. This approach not only enriches the understanding of ALD mechanisms but also sets a new standard for studying surface reactions in semiconductor fabrication.

Publication

G. D'Acunto, et al. Time evolution of surface species during the ALD of high-k oxide on InAs.

Surfaces and Interfaces 6, 17698 (2023).

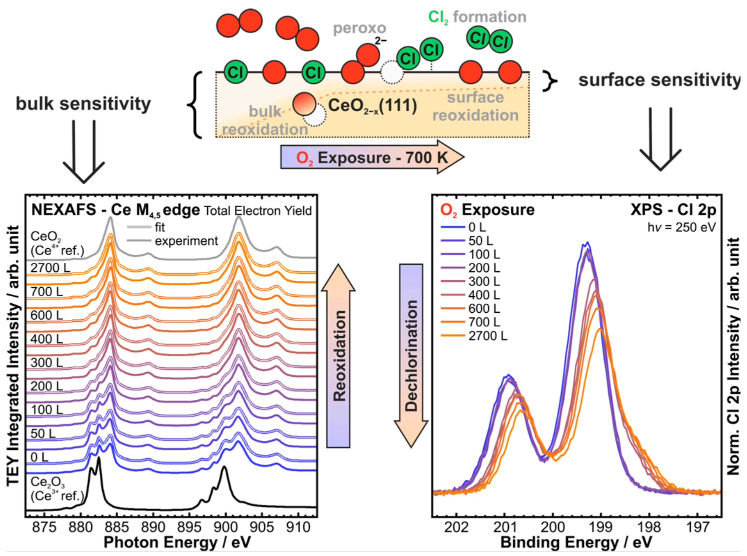
DOI: 10.1016/j.surfin.2023.102927

CATALYSIS

A sustainable process for chlorine recovery from hydrogen chloride

FlexPES

Chlorine is a valuable basic chemical that is essential for a broad range of products. However, hydrogen chloride is often an inevitable byproduct, accumulating to around ten million tons annually that are not used. A sustainable way to cope with this waste problem is to recover molecular chlorine by the Deacon process (2 HCl + O_2 –> Cl_2 + H_2O) over cerium dioxide catalyst. Compared to conventional hydrogen chloride electrolysis, only 15% of the energy is required.



XANES spectrum of bulk reoxidation, and surface dechlorination as a function of oxygen flow in Cl_2 production from HCl.

Researchers have used X-ray Photoelectron Spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) to study the reoxidation reaction in situ over a specifically designed model catalyst. They could disentangle the surface and bulk properties of the surface chlorinated model catalyst during the reoxidation process.

In a joined experiment and theory approach, they found the reoxidation process starts from the bulk of the catalyst and propagates towards the surface, very similar to filling up a glass of water. Strongly adsorbed chlorine recombines and forms the desired product Cl_2 only during surface oxidation.

The formation and dissociation of the peroxide species drive both processes, hence being considered essential for ceria-based catalysis in general.

Publication

V. Koller et al. Critical Step in the HCl Oxidation Reaction over Single-Crystalline CeO_{2-x}(111): Peroxo-Induced Site Change of Strongly Adsorbed Surface Chlorine.

ACS CATALYSIS 13, 12994 (2023).

DOI: 10.1021/acscatal.3c03222

CATALYSIS

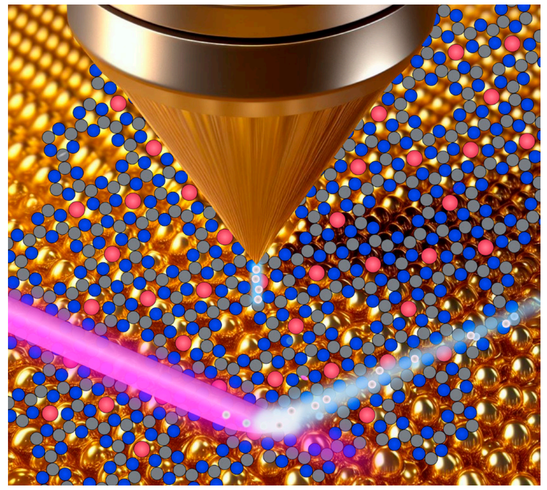
Synthesis and catalytic activity of a novel cobalt-doped carbon nitride material

FlexPES

Catalytic materials play an essential role for sustainable energy and transport in applications such as fuel cells. The Oxygen Reduction Reaction utilised in fuel cells can be catalysed by metal doped carbon nitrides.

A research team has created a graphitic carbon nitride (g-C_3N_4), on an Au(111) surface. g-C_3N_4 is a promising catalyst for a variety of reactions and a 2D material that has not been studied on a surface before. There has been a lot of debate over its exact structure and exposed catalytic sites in the literature. In this study cobalt and melamine react on an Au(111) surface to form a novel cobalt-doped carbon nitride. The research is a surface science study trying to elucidate the relationship between structure and reactivity of the novel and highly metal-rich carbon nitride. A planar model system is especially useful for this type of experiment.

The cobalt-doped carbon nitride showed excellent catalytic reactivity for the Oxygen Reduction Reaction. The study is also a framework for the investigation of similar materials in the future.



Scanning Tunneling Microscopy (STM) and X-ray PhotoElectron Spctroscopy were used to study the surface.

Publication

J. J. Gammelgaard et al. A Monolayer Carbon Nitride on Au(111) with a High Density of Single Co Sites.

ACS NANO 17, 17489 (2023).

DOI: 10.1021/acsnano.3c05996

CATALYSIS

Protective layer preserving catalyst material for energy conversion

HIPPIE

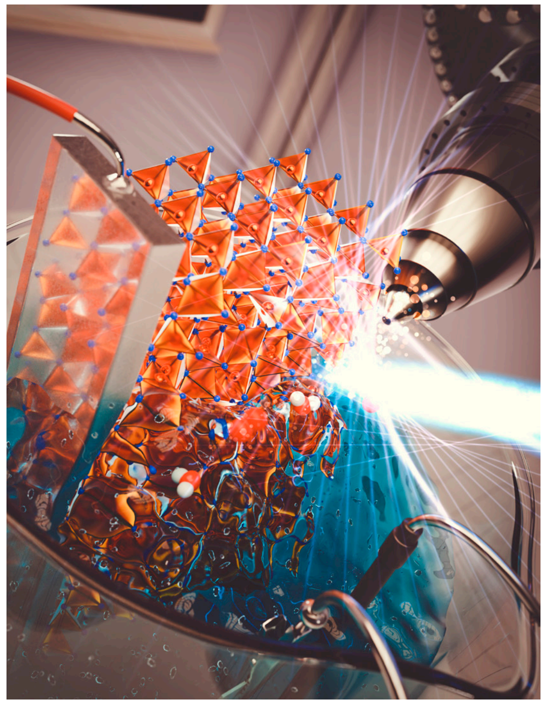


Photo-electrocatalyst at work studied with X-ray PhotoElectron Spectroscopy.

A team of Norwegian researchers has taken important steps towards development of a reliable photocatalyst for power-to-chemical applications. They have used a tantalum nitride, Ta_3N_5, photocatalyst and found how a nickel oxide coating, NiOx, can protect the surface against corrosion in harsh conditions.

Photocatalysts convert photons to electrons and holes, thus storing solar energy into chemical. One example is photo-electrolysis of water, where the catalyst materials absorb light to split water into hydrogen and oxygen. It is the "Holy Grail" of photocatalysis, a long running research field.

Some photocatalysts show high conversion efficiencies but they have poor stability. A protective coating of NiOx, an oxygen evolution reaction (OER) catalyst both helps with catalysis and protects the underlaying photocatalyst.

It is important to be able to test the photocatalyst in contact with water as this alters the band structure. The experiment is possible using the Ambient Pressure X-ray Photoelectron Spectroscopy technique. It resulted in mechanistic insights on the corrosion mechanism and under what conditions it can be avoided.

The researchers could measure electrical and spectroscopic properties of the material and found that the protective coating passivates surface states that would otherwise pin the Fermi level under light conditions and hinder the process of water photo-electrolysis.

Publication

Ø. Dahl et al. Interrogation of the Interfacial Energetics at a Tantalum Nitride/Electrolyte Heterojunction during Photoelectrochemical Water Splitting by Operando Ambient Pressure X-ray Photoelectron Spectroscopy.

ACS Catalysis 13, 11762 (2023).

DOI: 10.1021/acscatal.3c02423

CATALYSIS

Stabilising metal nanoparticles against sintering, a work towards more efficient catalysts

HIPPIE

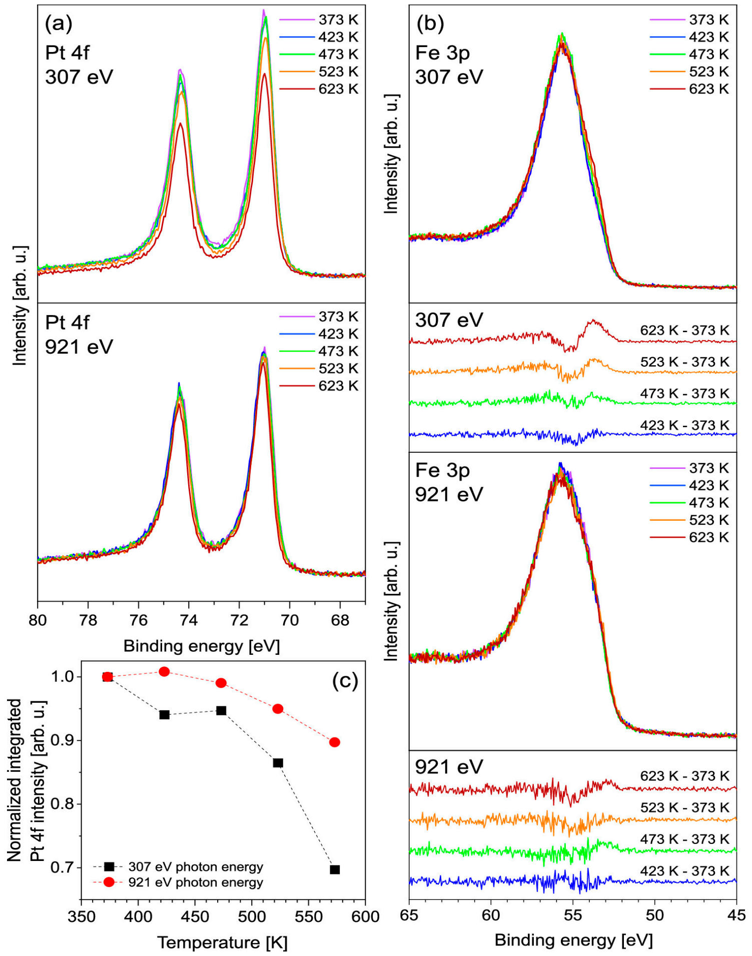
As highly active catalysts, the sintering of metal nanoparticles and sub-nm clusters into larger, less active particles often leads to a significant loss of their effectiveness at high temperatures. Researchers from the Technical University of Munich investigated whether encapsulating tiny Pt clusters with a very thin oxide layer can influence their dynamics and sintering behaviour during high-temperature catalysis through the so-called strong metal-support interaction (SMSI).

The research team combined several methods, namely scanning tunnelling microscopy (STM) for a structural investigation of the Pt clusters on Fe_3O_4(001) and a pulsed reactivity setup at the Technical University of Munich, and X-ray photoelectron spectroscopy at MAX IV.

The experiments showed that sub-nm clusters become encapsulated by the reducible oxide upon heating, while at the same time, two different sintering mechanisms set in, depending on cluster size.

More importantly, the sintering onset was pushed to significantly higher temperatures (823K) due to the encapsulating oxide layer – significantly higher than expected.

The possibility of stabilising highly active catalyst particles against deactivation aims to design more long-living catalysts and drastically reduce our need for valuable and rare noble metals, instead optimising their use through highly efficient chemical processes.



XP spectra of Pt_{19}/Fe_3O_4(001) (0.05 clusters/nm²) measured at 307 eV (highly surface-sensitive) and 921 eV photon energy (more bulk-sensitive), at the indicated temperatures in UHV. (a) Pt 4f spectra and (b) Fe 3p spectra with corresponding difference spectra for each photon energy below. (c) Evolution of the Pt 4f integrals for each photon energy, scaled to the first spectrum, respectively.

Publication

S. Kaiser, et al. Does Cluster Encapsulation Inhibit Sintering? Stabilization of Size-Selected Pt Clusters on Fe_3O_4(001) by SMSI.

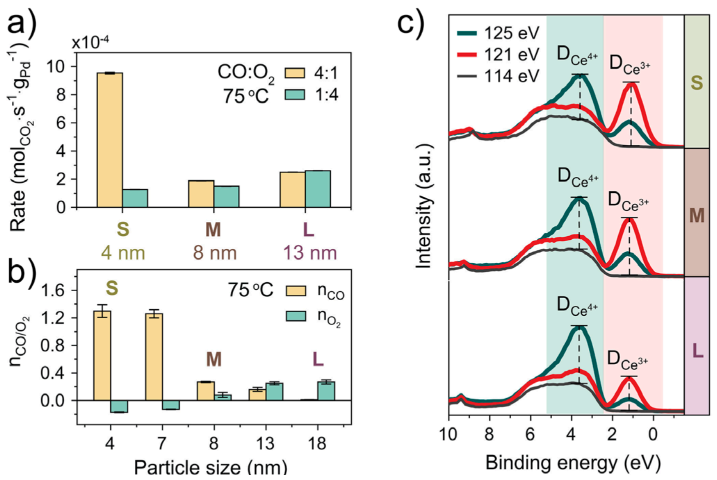
ACS Catalysis 13 (9), 6203-6213 (2023).

DOI: 10.1021/acscatal.3c00448

CATALYSIS

Tailoring properties of metal-based catalysts for exhaust treatment

Balder SPECIES



Size-dependent CO oxidation properties and reducibility in Pd/CeO_2 catalysts.

Researchers at Eindhoven University of Technology in the Netherlands explored new materials for three-way catalysts—devices used to clean toxic gases from gasoline vehicle exhaust. They studied the reactivity of palladium-cerium dioxide (CeO_2) composites, where palladium (Pd) is the active component and cerium dioxide stabilizes highly-dispersed Pd sites and provides oxygen storage capacity.

Results showed an unusual effect of CeO_2 particle size on the activity and stability of palladium species. Palladium supported on the smallest CeO_2 particles (4 nm) displayed excellent performance in a carbon monoxide (CO)-rich environment, while palladium atoms on a medium-sized support (8 nm) were highly active in a CO-depleted feed.

Additionally, the group found the particle size of CeO_2 strongly influences redox properties at the Pd-CeO_2 interface, with small particles exhibiting very high oxygen affinity. The analysis of Pd/CeO_2 material included measurements with X-ray absorption spectroscopy at MAX IV's BALDER beamline, and near ambient pressure X-ray photoelectron spectroscopy and resonant photoelectron spectroscopy at SPECIES beamline.

The work holds potential for the design of better catalyst for vehicle exhaust treatment and reduction of costly noble metals used for catalytic materials.

Publication

V. Muravev et al. Size of cerium dioxide support nanocrystals dictates reactivity of highly dispersed palladium catalysts.

SCIENCE 380, 1174 (2023).

DOI: 10.1126/science.adf9082

CATALYSIS

Promising rate-limiting step in Fischer-Tropsch synthesis with cobalt catalyst

FlexPES

Cobalt surfaces, which act as a catalyst for the production of synthetic fuels, will become very important for generating sustainable kerosene (SAF) for air transport. Cobalt is used in Fischer-Tropsch synthesis which can produce renewable hydrocarbons for the replacement of fossil fuel sources. Given this significance, researchers from company Syngaschem BV in the Netherlands used a combination of temperature-programmed desorption (TPD) and X-ray photoelectron spectroscopy (XPS) at FlexPES beamline to analyse how water and hydroxyl groups react on single-crystal surfaces of cobalt.

The study showed that hydroxyl intermediates quickly react to form water on flat surfaces and water does not dissociate on the surface.

Testing both flat and stepped surfaces, they sought to determine how the surface structure affects its reactivity.

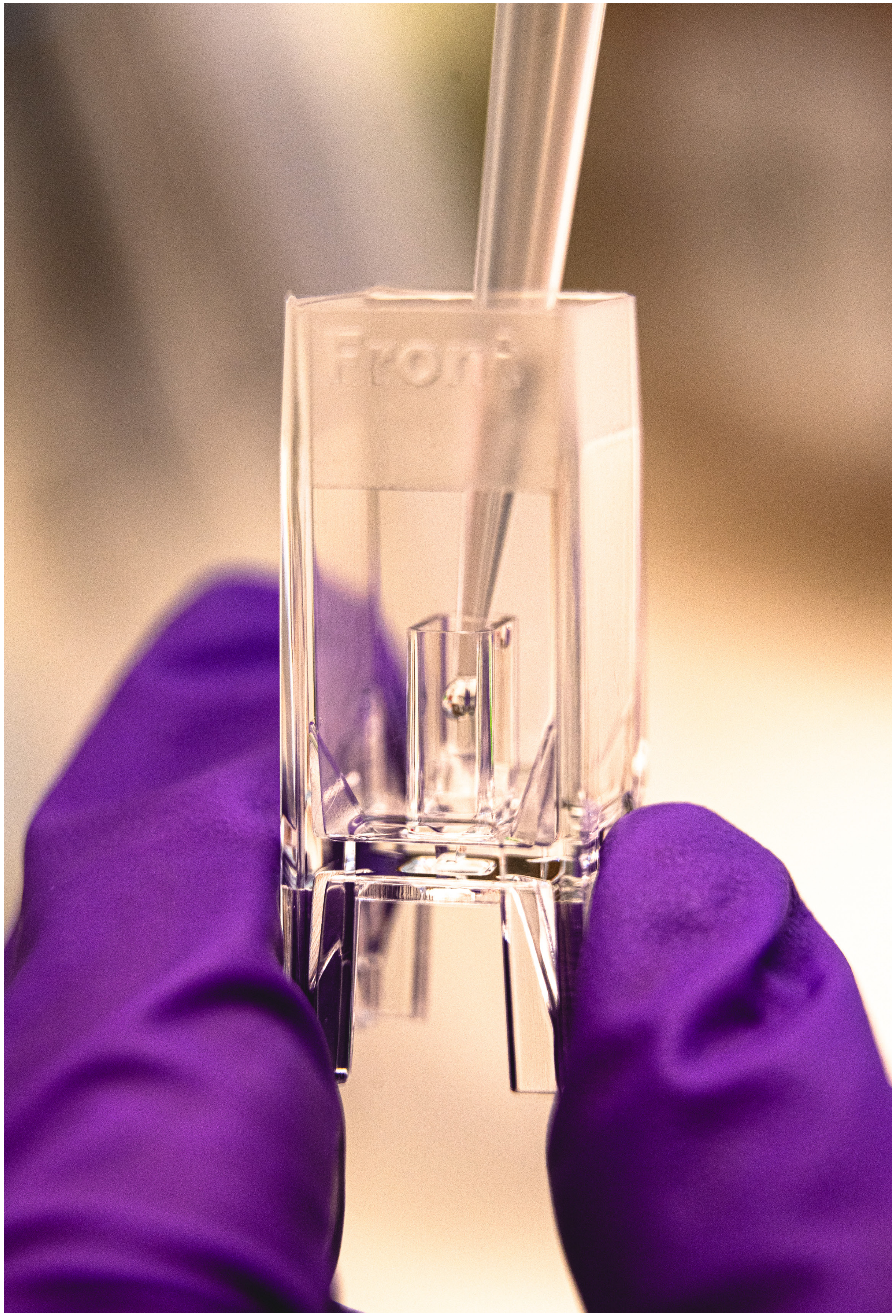
Results showed that hydroxyl intermediates quickly react to form water on flat surfaces and water does not dissociate on the surface. In contrast, these intermediates are much less reactive on stepped surfaces, and water dissociates easily on these surfaces. The study offers insight on the mechanism of water formation with cobalt catalysts, and whether this elementary step is rate-limiting in the catalytic reaction.

Publication

C.J. Weststrate et al. Water and Hydroxyl Reactivity on Flat and Stepped Cobalt Surfaces.

JOURNAL OF PHYSICAL CHEMISTRY C, 127, 2974-2980 (2023).

DOI: 10.1021/acs.jpcc.2c08425



ENERGY MATERIALS

On a quest to a more sustainable battery: Increasing Na-ion batteries efficiency

Balder

The scarcity of natural materials to produce the widely used Li-ion batteries has prompted researchers to find more sustainable alternatives. In the mission to provide a solution to this, the Ravnsbæk Group from Aarhus University studied Na-ion batteries at MAX IV.

Sodium batteries have a more promising future; they are abundant, economical, and have reduced environmental impact. However, structural distortions in layered $NaMO_2$ electrode materials are known to cause loss of capacity in Na-ion batteries with repeated cycling. Hence, scientists wanted to understand the structural distortions when the battery is in deep charge or discharge and how these transitions can be mitigated in materials with sustainable compositions, i.e., abundant materials such as Fe and Mn.

Drawing a complete structural evolution of the batteries during charge/discharge, the scientists discovered that increasing the amount of Fe in the material stabilises the pristine structure over a wide state-of-charge range.

Researchers employed operando powder X-ray diffraction (PXRD) at DanMAX and X-ray absorption spectroscopy at Balder to measure new sustainable electrode materials for Na-ion batteries, P_2-Nax-FeyMn$_1$−yO_2 (y = 0.33 and 0.5), putting focus on how the layered structure of the material changes as Na-ions are extracted and intercalated into the electrode during charge and discharge.

Using these methods, scientists could draw a complete structural evolution of the batteries during charge/discharge. Interestingly, it was discovered that increasing the amount of Fe in the material stabilises the pristine structure over a wide state-of-charge range: a new insight for a promising modification.

Publication

A. Ø. Drejer, et al. Local and Global Structures in the Phase Evolution of P2-NaxFeyMn1–yO2 Electrodes for Na-Ion Batteries.

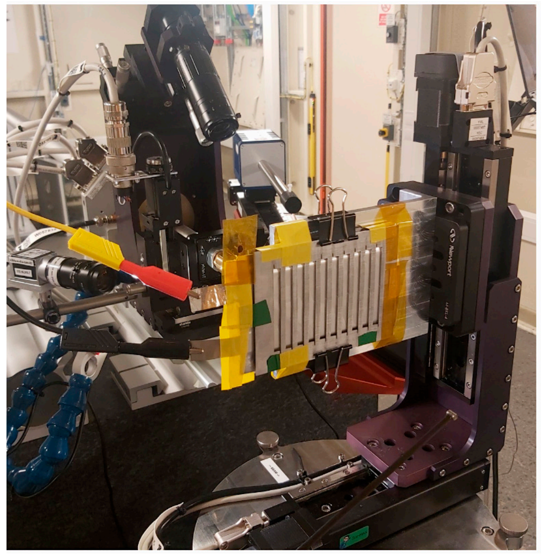
ACS Applied Energy Materials 6, 4909 (2023).

DOI: 10.1021/acsaem.3c00387

ENERGY MATERIALS

Revealing structural degradation for Li-ion batteries optimisation

DanMAX



Operando X-ray diffraction setup showing pouch cell clamped between two steel plates with ten cutouts at DanMAX beamline.

Improving the performance of Li-ion batteries by reducing degradation is a highly sought aim for expanded commercial use. Scientists at the Technical University of Denmark (DTU) performed an operando study of four prototype NMC811/Si–Gr 5Ah multilayered pouch cells (manufactured by Cidetec), a type of Li-ion battery. They endeavoured to understand the behaviour of Si–Gr (silicon graphite) anodes in conjunction with NMC811 cathodes.

Spatial and time resolved X-ray diffraction (XRD) measurements at MAX IV's DanMAX beamline were used to 2D-map the battery cathode and anode lithiation/delithiation, and volume expansion across the cell.

The tests provided information about structural changes during intercalation/deintercalation and spatial lithium inventory, and its relation to battery degradation. Results showed significant inhomogeneities across both electrodes, linked to volume expansion of the electrodes. Additionally, operando neutron diffraction analysis of the same prototype battery cells with Si-Gr anode following structural changes and phase transitions was done at the Paul Scherrer Institute (SINQ, PSI).

Real-time knowledge of reactions and materials transformation inside real battery geometries and how degradation relates to structural changes during battery use offers promise towards optimisation of rechargeable batteries.

The development of new high-performance batteries with a lower environmental footprint is important in the green transition to sustainable energy and transportation.

Publication

K.V. Graae et al. Time and space resolved operando synchrotron X-ray and Neutron diffraction study of NMC811/Si-Gr 5 Ah pouch cells.

Journal of Power Sources 570, 22993 (2023).

DOI: 10.1016/j.jpowsour.2023.232993

ENERGY MATERIALS

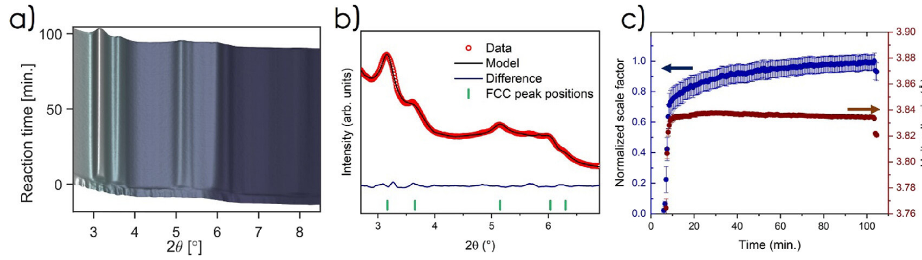
Replacing costly metals in catalytic particles for Power-to-X applications

DanMAX

High Entropy Alloy (HEA) Nano Particles are used as electrocatalysts for Power-to-X Applications, where sustainable energy is converted to fuels and chemicals as an essential part of the green transition.

A High Entropy Alloy consists of five or more components and has many interesting properties, such as many different adsorption sites at the surface. However, most High Entropy Alloys involve costly materials such as platinum, palladium, rhodium, iridium and ruthenium.

A Danish research team has previously developed a simple, green and scalable solvothermal synthesis method to obtain High Entropy Alloy Nano Particles of high homogeneity. In the present study, they explore the possibility of exchanging some of the expensive metals with cheaper so-called 3d-metals such as cobalt, nickel, and copper.



Results from the in situ X-ray scattering experiment on the formation of PtPdCuNiCo HEA nanoparticles. (a) Waterfall plot of the raw scattering data. (b) Obs–calc diagram after Rietveld refinement of one of the last diffractograms. (c) Extracted values after sequential Rietveld refinements: the normalized scale factor and the unit cell parameter. ***Credit:*** *Chem. Mater. 2023, 35, 1, 144-153.*

They show that it is possible to synthesise homogenous High Entropy Alloy Nano Particles containing eight metals, including the cheaper ones. The nanocrystal formation is studied using in situ Powder X-ray Diffraction and X-ray Atomic Pair Distribution Function.

Publication

N. L. Nyborg Broge et al, Facile Solvothermal Synthesis of Pt–Ir–Pd–Rh–Ru–Cu–Ni–Co High-Entropy Alloy Nanoparticles.

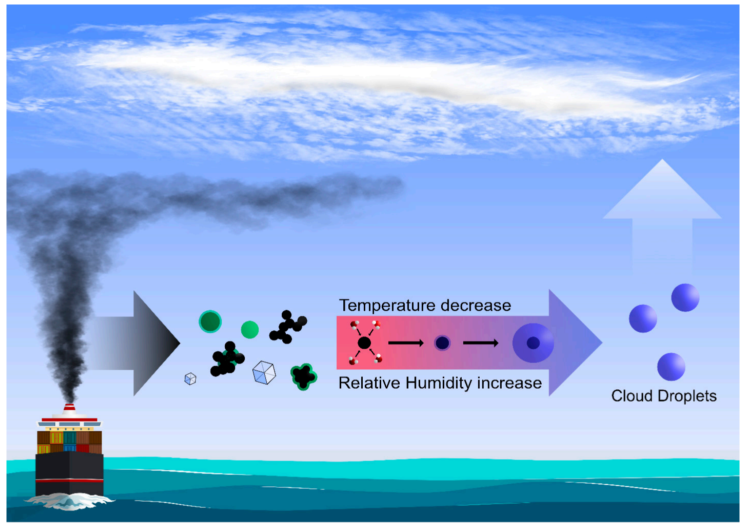
Chemistry of Materials 35, 144 (2023).

DOI: 10.1021/acs.chemmater.2c02842

ENVIRONMENTAL SCIENCE

A cloudy route for global shipping and climate

SoftiMAX



Cloud condensation nuclei (CCN) formation from ship emissions, depicting the transition from particulate emissions to aerosol particles and subsequent cloud droplet formation.

International maritime shipping regulations aim to reduce environmental impacts from sulphur emissions. Shippers can meet compliancy standards by use of sulphur removing devices, namely scrubbers, or low sulphur content (LSC) fuels. University of Gothenburg scientists analysed the cloud-forming abilities of particle exhaust from ships using low-sulphate fuels and high-sulphate fuels conditioned with wet scrubbers. Cloud condensation nuclei (CCN) activity was measured with scanning transmission X-ray microscopy (STXM) at SoftiMAX beamline.

The group found that high sulphate fuel with scrubbers consequentially produced more cloud condensation nuclei or cloud seeds, and emissions with hygroscopic particles. Hygroscopic particles which absorb water from the air (cloud formation), can increase cloud albedo, and extend cloud lifetime or increase precipitation.

Further, switching to LSC fuels can significantly reduce ultrafine particulate matter emissions, which leads to a significant decrease of particle number emissions, primarily due to the absence of sulphate-rich particles. The reduction affects CCN activity of exhaust particles, resulting in decreased emissions of cloud-forming particles.

The findings suggest that while both LSC fuels and exhaust wet scrubbing reduce total particle emissions, they have opposing effects on the emissions of cloud-forming particles, with significant implications for maritime shipping impacts on the environment and climate.

Publication

L. Santos et al. Changes in CCN activity of ship exhaust particles induced by fuel sulfur content reduction and wet scrubbing.

ENVIRONMENTAL SCIENCE: ATMOSPHERES 3, 182 (2023).

DOI: 10.1039/D2EA00081D

ENVIRONMENTAL SCIENCE

Seeking utility in toxic groundwater treatment waste

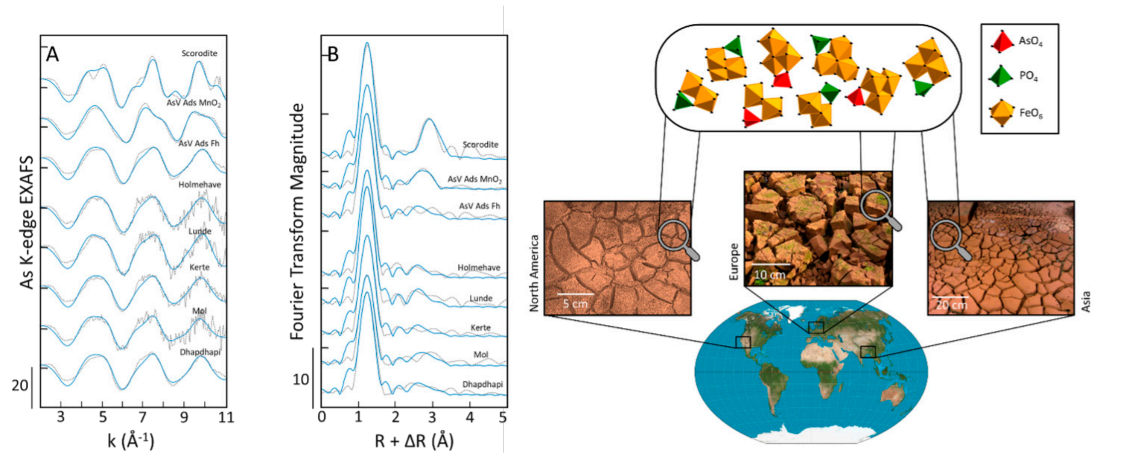
Balder

The European Commission listed arsenic (As) as a Critical Raw Material (CRM) in 2023. Arsenic is a key component of alloys, batteries, and high-speed electronics, and interest has increased significantly for upcycling the toxic element from As-rich groundwater treatment waste. As waste is typically considered a disposable bi-product.

Scientists at the Geological Survey of Denmark and Greenland sought to identify the solid-phase speciation of arsenic (As) and iron (Fe) in sludge created from As-removal in groundwater in many different affected regions. The samples were measured using X-ray absorption spectroscopy (XAS) at MAX IV's Balder beamline.

The results showed that bonding environments of As and Fe in a range of sludge samples were essentially identical, with all samples consisting of arsenate (As(V)) bound in the binuclear-corner sharing (2C) geometry to highly disordered Fe(III) precipitates. The findings demonstrate As recovery methods optimised for one type of treatment sludge can be applied universally to other types, regardless of raw groundwater composition, treatment mechanism, geographic region or other variations.

The study advances knowledge for the design and optimisation of novel conversion techniques for As-treatment sludge to valuable materials for a circular economy.



Arsenic K-edge EXAFS spectra (A) and corresponding Fourier transforms (B) for As-rich waste samples collected from groundwater treatment plants around the world.

Publication

K. Wang et al. Molecular-scale characterization of groundwater treatment sludge from around the world: Implications for potential arsenic recovery.

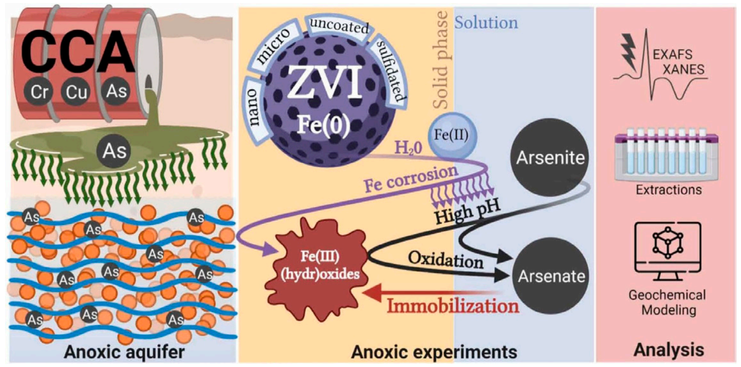
WATER RESEARCH 245, 120561 (2023).

DOI: 10.1016/j.watres.2023.120561

ENVIRONMENTAL SCIENCE

Removing arsenic from groundwater using zero-valent iron particles

Balder



Experiments, data analysis and modelling lead to zero-valent iron particles that can be used to immobilise arsenic in groundwater.

Arsenic poses a threat to human health, and the WHO considers groundwater the riskiest source for human intake of arsenic. However, dealing with arsenic contamination remains a scientific challenge. A team led by researchers based at SLU, Uppsala, have recently provided a strong geochemical background for the application of zero-valent Iron particles to remove arsenic from contaminated aquifers.

They tested different zero-valent iron particles in a contaminated site of a former wood impregnation plant in Småland, Sweden. Thanks to their efforts in maintaining field-realistic conditions throughout the study, they unveiled immobilisation mechanisms for arsenic that could not be previously demonstrated using simplified laboratory conditions.

The study found that, despite the lack of oxygen in the aquifer, zero-valent iron promotes arsenic retention via an oxidation mechanism involving Iron corrosion and a sharp increase in pH. As a result, the coating structure of the zero-valent Iron particles had a greater effect on the arsenic immobilisation performance when compared to the initial size of the zero-valent iron particles.

Publication

T. A. Formentini et al. Immobilizing arsenic in contaminated anoxic aquifer sediment using sulfidated and uncoated zero-valent iron (ZVI).

Journal of Hazardous Materials 462, 132743 (2024).

DOI: 10.1016/j.jhazmat.2023.132743

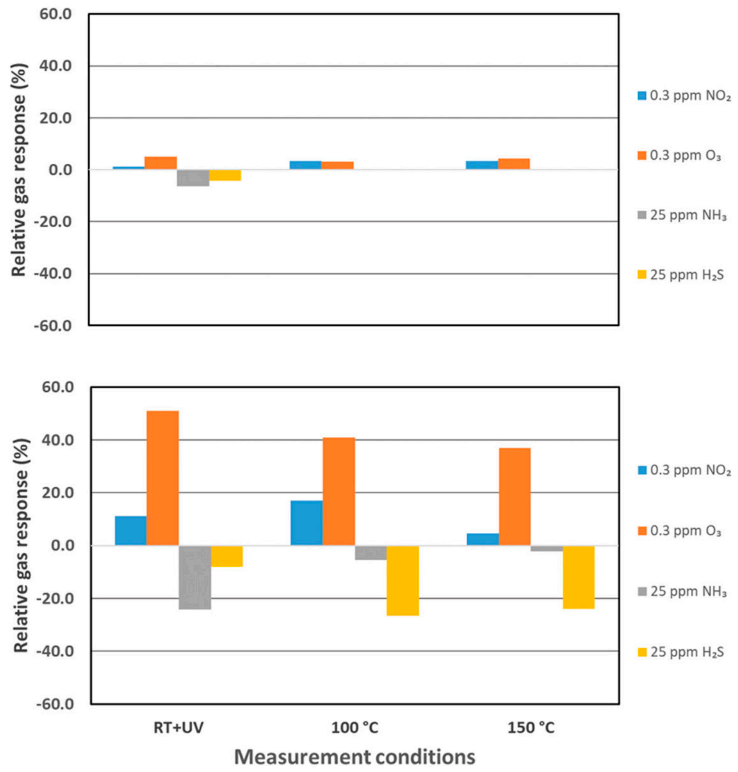
Oxide layer increases chemical sensitivity of graphene for e-nose applications

FinEstBeAMS

A low-cost, miniature, low-energy consumption so-called electronic nose could be used to monitor indoor and outdoor air quality. It would be of immense importance as a tool to control the health effects originating from poisonous gases.

A team of researchers from Estonia are working towards finding materials to functionalise graphene gas sensors to make them more responsive towards polluting gases. Graphene is sensitive towards perturbations to its' surface and, therefore, a great candidate for sensing. In this study, they used a $CuMn_2O_4$ deposition source to deposit a mixed copper/manganese-oxide layer onto the graphene.

After the oxide deposition, the sensor's responses towards gases increased significantly. The responses also depend strongly on measuring temperature – so the sensor selectivity is induced by functionalising the oxide layer. The researchers measured the gas responses towards several polluting gases: NO_2, O_3, H_2S, and NH_3. The partial gas selectivity gives great promise to use this functionalising material and graphene combination in electronic noses.



Response of the electronic nose to different gasses and conditions.

Publication

M. Kodu. Gas-Sensing Properties of Graphene Functionalized with Ternary Cu-Mn Oxides for E-Nose Applications.

Chemosensors 11, 460 (2023).

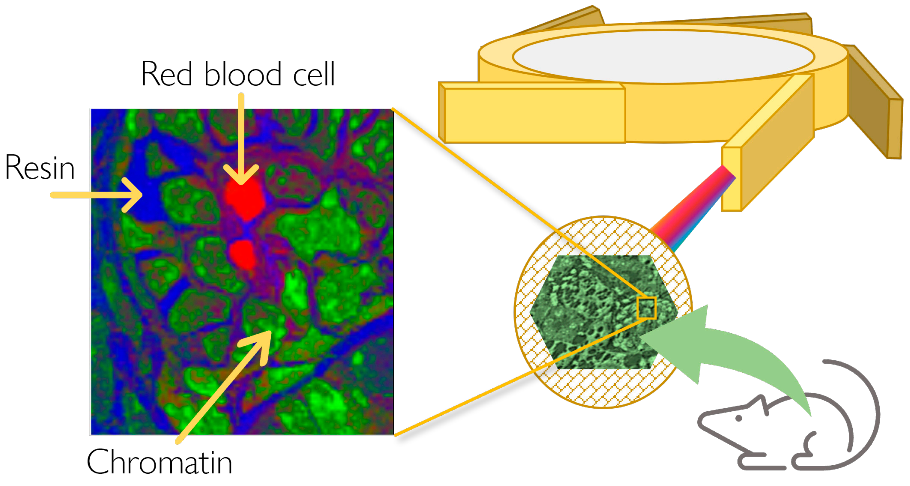
DOI: 10.3390/chemosensors11080460

HEALTH AND MEDICINE

In its purest form: STXM study on lysosomal storage diseases

SoftiMAX

Exploring novel methods to study the characterisation and accommodate further understanding of lysosomal storage diseases (LSDs), researchers from the University of Oulu, in collaboration with the FinnDisMice consortium, conducted a scanning transmission X-ray microscopy experiment at MAX IV (SoftíMAX beamline) and UVSOR III (BL4U) with complementary electron microscopic data at Biocenter Oulu on kidney and liver tissues of gene-edited mice. LSDs are rare disorders where some material accumulates in cells due to dysfunction in enzymes which are responsible for the transport or catabolism of macromolecules. The LSD chosen for this study is Salla disease, in which sialic acid builds up in lysosomes.



By using STXM method at SoftiMAX, samples from mice with salla disease have higher contrast make it possible to study them on its purest form. ***Credit:*** *Minna Patanen.*

As a result, the STXM method showed natural chemical contrast in samples, eliminating the need for staining agents and maintaining the specimen to its purest form for observation. Researchers focused on the rapidly varying absorption contrast between different cell organelles. They can see that the developed mouse model expressed changes in the tissues similar to those reported in patients with LSD.

The successful experiment will contribute to future development of diagnostics and novel treatments for LSDs.

Publication

T. Mansikkala, et al. Scanning transmission soft X-ray spectromicroscopy of mouse kidney and liver.

Journal of Electron Spectroscopy and Related Phenomena 266, 147368 (2023).

DOI: 10.1016/j.elspec.2023.147368

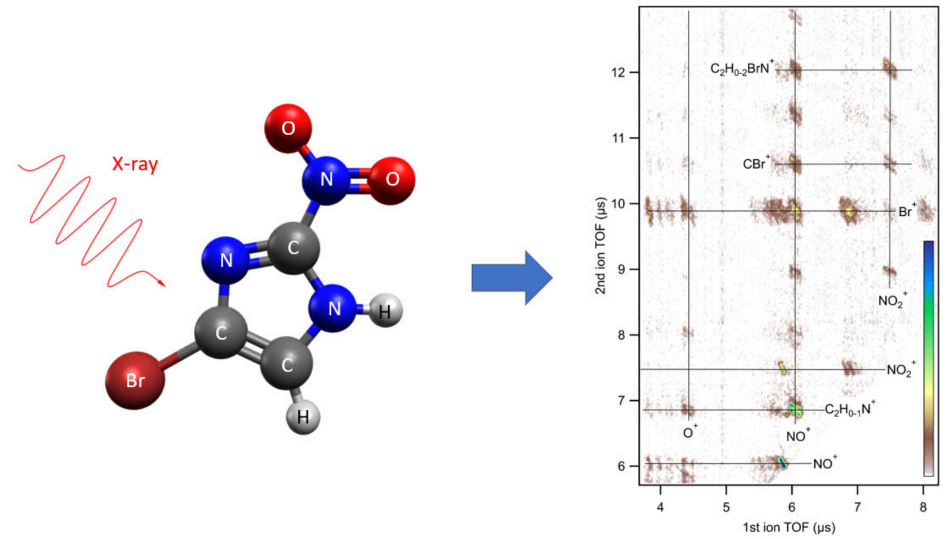
HEALTH AND MEDICINE

New fundamental understanding of radiosensitisers to improve cancer treatment

FinEstBeAMS

Radiotherapy for cancer treatments involves ionising radiation, and improving its selectivity to better target malignant cells during the radiation treatment has been researchers' focus for a long time. Among others, this can be achieved by using radiosensitisers, e.g., nitroimidazoles or heavy elements, which can enhance radiotherapy's effectiveness. An international collaboration led by researchers from the University of Turku tapped into the unknown territory of molecular-level radiosensitisation mechanisms of halogenated nitroimidazoles.

The research was done at FinEstBeAMS beamline using the photoelectron-photoion-photoion coincidence spectroscopy (PEPIPICO) technique to investigate the impact of bromination on the photodissociation dynamics of nitroimidazole. The focus was on the fragmentation of two brominated samples and a bromine-free reference upon ionisation of Br 3d, C 1s, and N 1s. A comparison with the non-brominated reference revealed that, although the bromination slightly inhibited the charge localisation on the nitro group, the dissociation of the brominated samples resulted in a significant release of fragments that could cause cellular damage.



Employing the PEPIPICO technique at FinEstBeAMS, core-ionised brominated nitroimidazoles were shown to release O+, NO+, NO_2+, and Br+ upon dissociation, which could cause increased cellular damage in cancer treatments. ***Credit:*** *Lassi Pihlava.*

The research gives new insights into how nitroimidazoles respond to photoionisation and further studies on halogenated nitroimidazoles continue. This fundamental finding can aid in the pursuit of future new, more potent radiosensitiser drugs for cancer radiotherapy.

Publication

L. Pihlava, et al. Photodissociation of bromine-substituted nitroimidazole radiosensitizers.

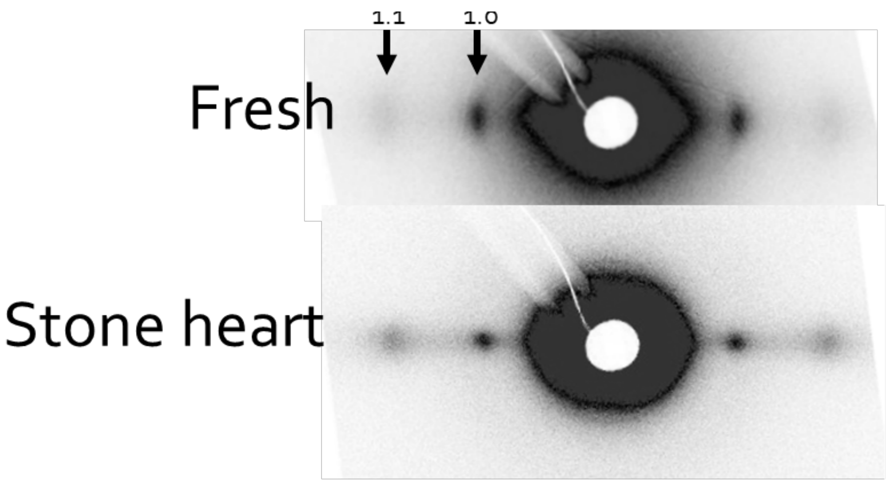
Physical Chemistry Chemical Physics 25, 13004 (2023).

DOI: 10.1039/D2CP04888D

In search for insights into stone heart syndrome

CoSAXS

More than a thousand patients stand on the waiting list for heart transplantation in Europe alone. Once granted, their chance of getting a heart transplant is dependent on whether the donor's heart is suitable and in good condition. Ischemic injuries are always a threat - a condition caused by long exposure to warm ischemia (state without metabolic supply), known as 'stone heart' syndrome. Ischemic injury and the irreversible contracture of the heart make it impossible to perform a successful heart transplantation.



Equatorial X-ray scattering patterns from a normal/fresh heart and a heart with ischemic contracture (stone heart). In the stone heart, the spacing of the 1.1 and 1.0 reflections is unchanged, suggesting unchanged filament distances, but the intensity of the outer 1.1 reflections is increased, suggesting mass transfer between contractile filaments.
***Credit:** Anders Arner.*

To understand the underlying mechanism and aim to prevent 'stone heart', researchers from Igelösa Life Science and the Department of Clinical Sciences Lund worked with pig hearts that have strong similarities with the human heart and have recently been used for xenotransplantation. They ask: Is the filament lattice shrinking in the ischemic contracture? Does the contracture involve attachment/mass transfer between the contractile filaments?

Using small-angle X-ray scattering at CoSAXS, researchers found that the contracture does not involve shrinkage of the contractile apparatus and is associated with interactions between the contractile filaments instead. Understanding ischemic contracture gives information on pathological changes that can occur in the cardiac muscle. Researchers recently developed a potential approach to inhibit the ischemic contracture. Further research at MAX IV is in the pipeline.

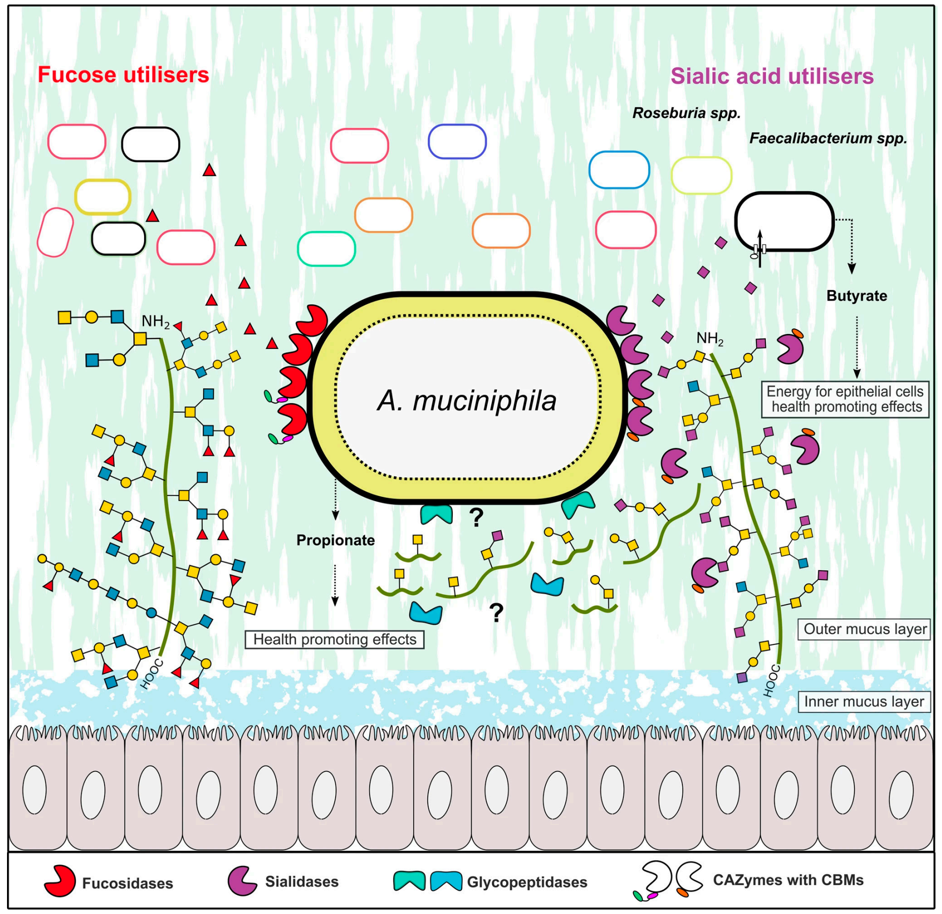
Publication
M. Li, et al. Development and prevention of ischemic contracture ("stone heart") in the pig heart.
Frontiers in cardiovascular medicine 10, 1105257 (2023).
DOI: 10.3389/fcvm.2023.1105257

Gut health: Unlocking the strategy of a key bacterial symbiont

BioMAX

Scientists are interested in the symbiont gut bacterium, Akkermansia muciniphila, for its beneficial impact on human immune modulation, body weight, and metabolic markers. Its abundance is linked to favourable metabolic health and gut barrier function, while reduced abundance is observed in dysbiotic disease-associated microbiota. Seeking to understand the strategies by which A. muciniphila nourishes itself in the gut lining and impacts other beneficial gut symbionts, a research group from the Technical University of Denmark (DTU) investigated ten enzymes of the bacterium that enable its interaction with mucin, the structural scaffold of the gut mucosa.

Results show A. muciniphila fucosidases and sialidases initiate the breakdown of mucin by decapping mucin O-glycans, consequently allowing 'soft' cleavage of the mucosal backbone by specialized mucinases. This mediates nutrient-sharing with other mucus-associated microbiota on the lining. Diffraction data of the complex fucosidase AmGH29D was obtained at MAX IV's BioMAX beamline. The study advances knowledge of A. muciniphila and other beneficial gut bacteria, which are emerging probiotic candidates for therapeutic treatment of lifestyle diseases including obesity and metabolic syndrome.



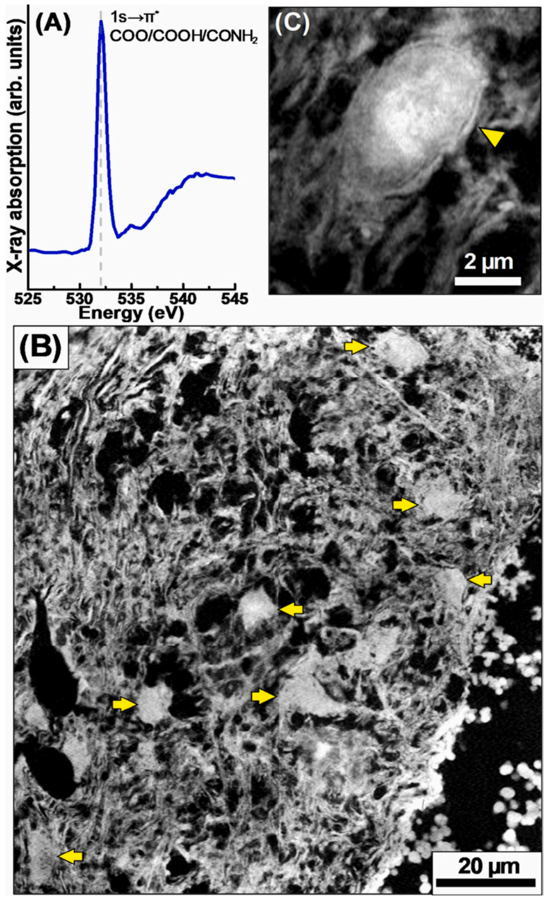
Model for mucin defucosylation and desialylation by A. muciniphila and sharing of fucose and sialic acid with mucus adherent butyrogenic gut microbiota.

Publication
B. Shuoker et al. Sialidases and fucosidases of Akkermansia muciniphila are crucial for growth on mucin and nutrient sharing with mucus-associated gut bacteria.
Nature Communications 14, 1833 (2023).
DOI: 10.1038/s41467-023-37533-6

Illuminating brain biochemistry to understand disease

SoftiMAX

Comprehensive knowledge of fundamental chemical processes of the healthy and diseased human brain is yet to be realized. With millions afflicted by Alzheimer's and Parkinson's disease worldwide, studies are vital to pinpoint disease mechanisms and changes which occur during the course of disease. To explore the biochemical composition of postmortem brain tissue from neurologically healthy individuals, and individuals afflicted by neurodegenerative disease, researchers from Keele University and the University of Warwick in the United Kingdom utilized scanning transmission X-ray microscopy (STXM) at MAX IV's SoftiMAX beamline.



Data of chemically-sensitive images and detailed X-ray absorption spectra to a spatial resolution of approximately 50 nanometres revealed the distribution of different biochemical constituents and chemical states of elements within the samples in highly localized brain regions of interest. With STXM measurements of Alzheimer's disease tissue, the group made an unexpected discovery of elemental metallic copper and ferromagnetic iron nano-deposits associated with pathological features of the disease, which were previously undocumented in the human brain. The X-ray analysis offers new insights into neurochemistry, neurobiology, and the etiology of neurodegenerative diseases, which could open paths for improved diagnostic techniques and efficacious treatments.

Carbon K-edge STXM data from hippocampus and amygdala tissue sections from two Alzheimer's disease cases, and the substantia nigra of a Parkinson's disease case.

Publication

J. Everett et al. Illuminating the brain: Revealing brain biochemistry with synchrotron X-ray spectromicroscopy.

JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA 266, 147355 (2023).

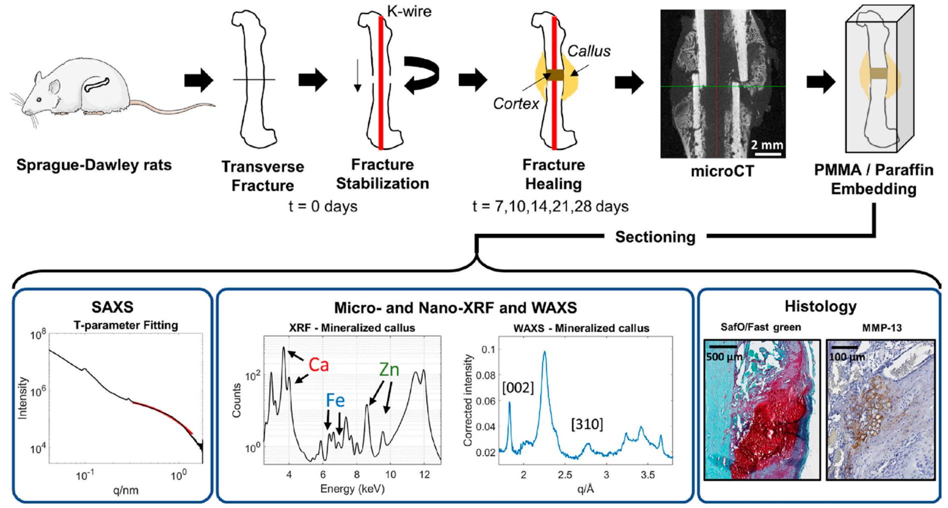
DOI: 10.1016/j.elspec.2023.147355

A nanoscale view of mineralisation in bone fracture healing

NanoMAX

Bone mineralisation involves a complex coordination of physico-chemical processes, and the mineralisation mechanisms remain elusive for science. Biomechanics and orthopaedics researchers at Lund University characterised the relationship between structural changes and the presence of different chemical elements and compounds during the stages of in-vivo long bone fracture healing. Nano X-ray fluorescence (XRF) and wide-angle X-ray scattering (WAXS) measurements were made at NanoMAX beamline at MAX IV.

The research group correlated the spatio-temporal distribution of trace elements to the deposition and maturation of hydroxyapatite nanocrystals and the presence of matrix remodelling compounds (MMP-13). Multi-scale measurements indicated that calcium, zinc and iron act in coordination for both the initial mineral deposition and resorption processes during mature mineral remodelling. Zinc and MMP-13 showed similar spatio-temporal trends during early mineralisation.



Methodology and techniques used in the characterisation of different stages in endochondral fracture healing.

The results lend new evidence for the time-events and interplay between elements. The study advances understanding of component linkages in the bone mineralisation process—important for the elucidation of its mineralisation mechanisms and ultimately, future development of targeted treatments for bone fracture healing.

Publication

D. Hector et al. Multi-scale characterization of the spatio-temporal interplay between elemental composition, mineral deposition and remodelling in bone fracture healing.

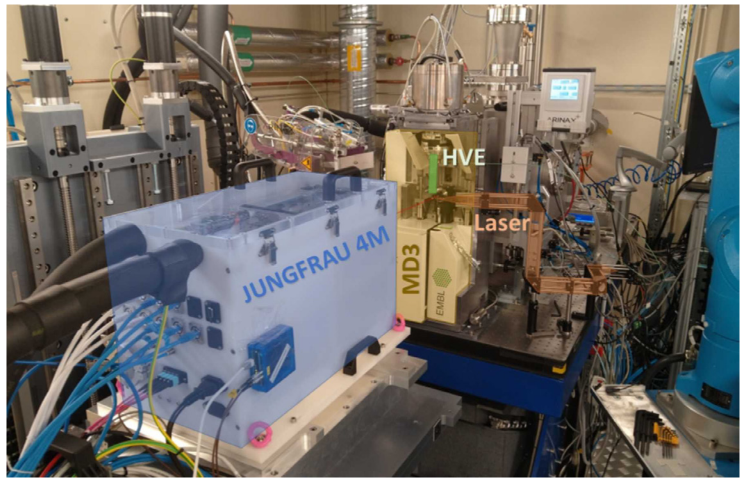
Acta Biomaterialia 167 (2023).

DOI: 10.1016/j.actbio.2023.06.031

Serial and time-resolved macromolecular crystallography setup for next-level structural biology research at MAX IV

BioMAX

To reap MAX IV's full potential as the world's first 4th generation synchrotron source, a collaborative work between researchers from the Paul Scherrer Institute and MAX IV experimented on a serial and time-resolved macromolecular crystallography setup. The new setup aimed to fill the gap in structural biology research and made it possible to follow proteins' processes and dynamics in a moving picture. The setup makes it possible for a new chapter of structural biology research, including ultra-high-throughput screening, serial crystallography structure determination of true microcrystals, and especially time-resolved MX.



The setup at the BioMAX beamline. Blue represents the JUNGFRAU 4M prototype detector, yellow is the existing MD3 diffractometer, orange is the transient laser triggering setup and green is the mounted HVE.

Scientists set up the PSI-developed adaptive-gain charge-integrating JUNGFRAU detector and Jungfraujoch server for detector control and data readout at BioMAX. They observed the dynamics of lysozyme microcrystals and the light-driven sodium-pump membrane protein KR2. As a result, the researchers gathered a molecular moving picture of up to 500 microseconds in resolution of the protein dynamics, providing ten times finer details than the previously available method.

The collaborative work continues, and the setup will be available at MicroMAX beamline for MAX IV users.

Publication

F. Leonarski, et al. Kilohertz serial crystallography with the JUNGFRAU detector at a fourth-generation synchrotron source.

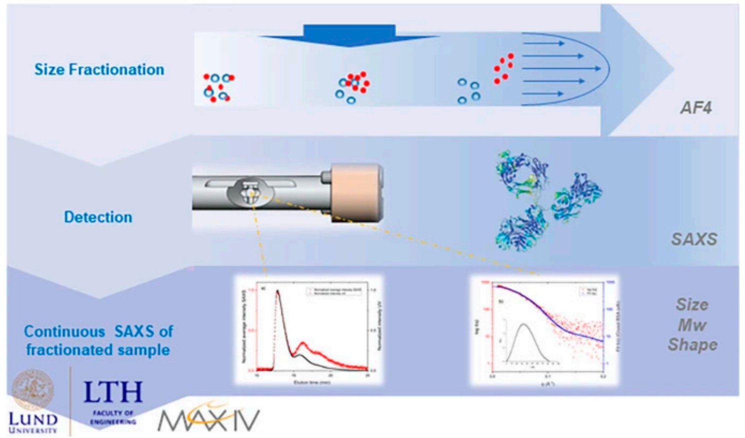
IUCrJ 10, 729 (2023).

DOI: 10.1107/S2052252523008618

New AF4-UV-SAXS method for studies of complex biomolecules and biologics

CoSAXS

Researchers from Lund University evaluated a new method for the study of sensitive and complex samples and pharmaceutical formulations using small-angle X-ray scattering (SAXS) or BioSAXS.



New method AF4-UV-SAXS combines SAXS and asymmetrical flow field flow fractionation for study of biomolecules.

A first of its kind, method AF4-UV-SAXS is a direct, on-line coupling of asymmetrical flow field flow fractionation (AF4)—a separation technique for colloidal samples and biomolecules in solution—and synchrotron SAXS. The proof of concept was confirmed with essential high flux measurements of the bovine serum albumin (BSA) protein and a monoclonal antibody (mAb) at MAX IV's CoSAXS beamline.

Results revealed that even low concentrations eluting from the AF4 separation device were sufficient to produce adequate scattering from the low electron density biomolecule samples. The NextBioForm/VINNOVA study demonstrates the feasibility of the AF4-UV-SAXS method for the study of complex biomolecule assemblies, and in connection, holds potential for future development of stable and improved biologics for patient care.

Publication

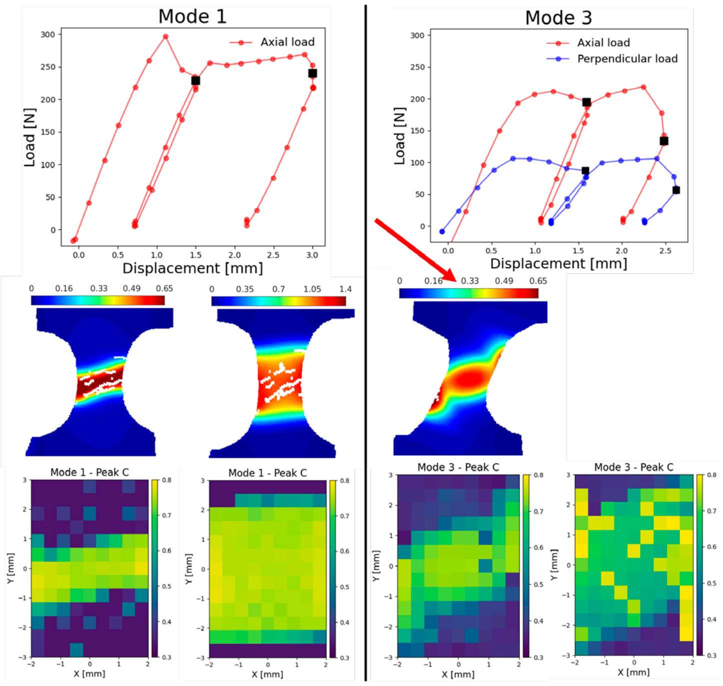
H. Bolinsson et al. Realizing the AF4-UV-SAXS on-line coupling on protein and antibodies using high flux synchrotron radiation at the CoSAXS beamline, MAX IV.

ANALYTICAL AND BIOANALYTICAL CHEMISTRY 415, 6237 (2023).

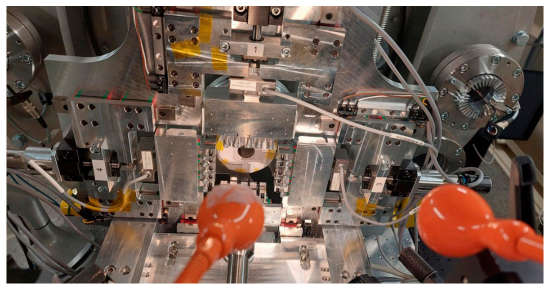
DOI: 10.1007/s00216-023-04900-7

New setup for mechanical testing of composite and polymer materials

CoSAXS



Measured load-displacement curves.



Experimental setup.

Composite and polymeric materials are used in a vast range of applications, often where weight reduction is relevant while maintaining a good mechanical performance. They are relevant for packaging solutions, aerospace applications or in wind turbines, among others. A systematic study of such materials is important for the design, testing and development of novel solutions.

A collaboration between the CoSAXS beamline at MAX IV and the department of Solid Mechanics at Lund University lead to a tailored solution for mechanical testing. The design favours simultaneous measurement of small- and wide-angle X-ray scattering for multiscale investigations of the material under load. It allows multiple deformation modes and is compatible with 3D-surface image correlation for spatially resolved mesoscopic surface deformation.

The setup has been used to characterise the structural evolution of polymer materials relevant to industry, such as polycarbonate and polyethylene. The research team has characterised the deformation of the different elements of the polymeric chain for polycarbonate, following the formation and development of cracks before failure. For polyethylene, they have locally induced the transition between the orthorhombic to monoclinic phase due to local stress concentration. For carbon fibre, they followed the elastic deformation of the crystalline structure, and the defects present in the hierarchical structure.

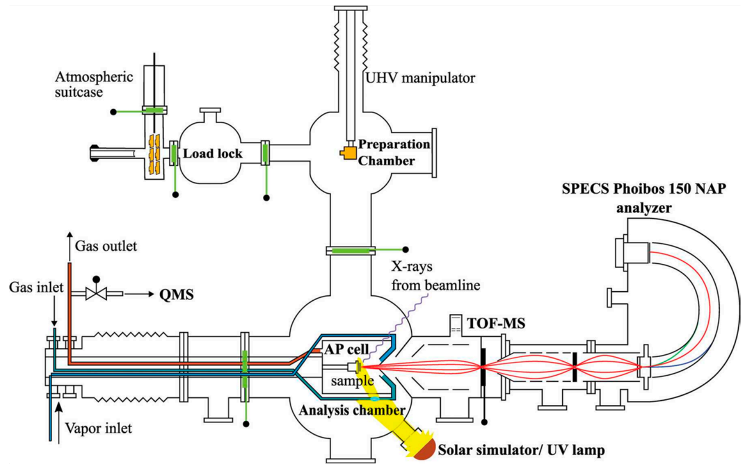
Publication

P. Mota-Santiago et al. In situ biaxial loading and multi-scale deformation mesurements of nanustructured materials at the CoSAXS beamline at the MAX IV Laboratory.
Journal of Applied Crystallography 56, 967 (2023).
DOI: 10.1107/S1600576723005034

Photocatalytic setup for in situ and operando Ambient Pressure X-ray Photoelectron Spectroscopy

SPECIES

The capabilities of the Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) endstation at the SPECIES beamline have been extended by a novel photocatalytic setup. The instrumentation allows the study of solar radiation-driven processes by combining external light sources with the APXPS measurements. In situ and operando experiments can be carried out with the setup under mbar pressure ranges, which often approach realistic scenarios in either industry or nature. The development of the setup is the result of a collaboration between MAX IV and the University of Oulu, Finland.



Schematic of the experiment setup.

As a case study, we have investigated the photocatalytic hydrogen evolution reaction, which is a promising technique for harvesting and storing solar energy into chemical energy and has been studied for decades.

Here, a special core-shell photocatalyst comprising of Ni metal inside a NiO/$NiCO_3$ nanoparticle was investigated as it was immersed in water vapour and exposed to solar radiation. It was discovered that the photocatalyst exhibits specific structural and electronic changes upon reactions with water and solar radiation. For example, the nickel oxide is reversibly transformed into nickel hydroxide.

This works highlights the uniqueness of APXPS in this study and how it can be used to study the charge transfer dynamics, which is important for further development of the photocatalysts with improved characteristics.

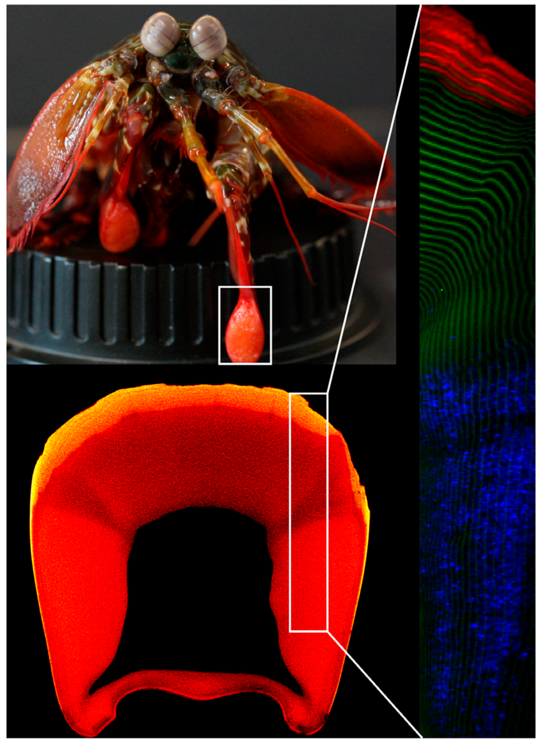
Publication

A. Klyushin et al. Photocatalytic setup for in situ and operando ambient-pressure X-ray photoelectron spectroscopy at MAX IV Laboratory.
Journal of Synchrotron Radiation 30, 613 (2023).
DOI: 10.1107/S1600577523002801

STRUCTURAL BIOLOGY

Extreme marine anatomy inspires for functional materials design

DanMAX



Mantis shrimp with dactyl club (shown in rectangle), including virtual slice with 3D X-ray microscopy data.

Mantis shrimp hunt prey using large hammer-like appendages called dactyl clubs. Mollusc shells are effectually broken with a combination of ultrarapid impact and the dense, biomineralized club structure of chitin and apatite crystallites.

A research group from Aarhus University in Denmark investigated the side of the club, known as the periodic and striated regions, typically composed of amorphous mineral phases.

Results showed that minerals transition here from an amorphous to a crystalline phase, calcite ($CaCO_3$), in varying degrees in some clubs. This indicates useability in the club in either phase, and a flexibility in the club design which enables structural evolution. Additionally, large crystallites were observed to organize around chitin bands, suggesting chitin may serve as a template for crystallisation. The stomatopod clubs were measured with scanning X-ray diffraction (XRD) in part at MAX IV's DanMAX beamline.

The study advances understanding of extreme hierarchical structures in biological materials and holds promise for the potential design of bioinspired synthetic functional materials.

Publication

T.E.K. Christensen et al. Flexible design in the stomatopod dactyl club.

IUCrJ 10, 288-296 (2023).

DOI: 10.1107/S2052252523002075

STRUCTURAL BIOLOGY

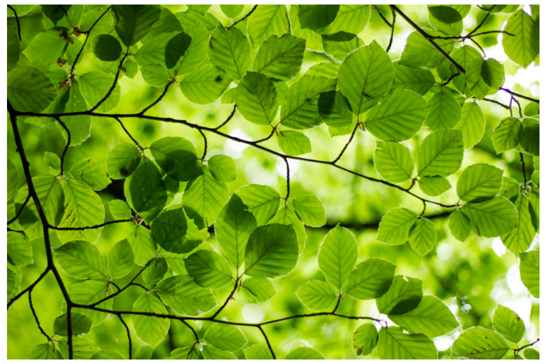
Decoding growth – uncovering sucrose transport in plants

BioMAX

Researchers have determined the structure of the SUC1-protein situated in the cell membrane and is essential for active sucrose transport in plants. Sucrose is a sugar and a product of photosynthesis. It plays a key role in growth as a building block for new molecules and a crucial energy source for the plant cells.

Uncovering the structure of SUC1 and understanding how it recognizes sucrose and facilitates proton-coupled transport is a significant insight into the process of nutrient transport in plants. Sucrose transport and loading into the phloem, the vascular tissue of plants, affect turgor pressure, vascular nutrient flow, and, ultimately, growth and morphology.

The result therefore has potential applications in agriculture and plant manipulation and opens avenues for future advances in enhancing crop growth and adapting plants to environmental challenges.



Understanding how SUC1 recognises sucrose and facilitates proton-coupled transport is a significant insight into the process of nutrient transport in plants.

Publication

L. Bavnhøj at al., Structure and sucrose binding mechanism of the plant SUC1 sucrose transporter.

Nature Plants 9, 938 (2023).

DOI: 10.1038/s41477-023-01421-0

An experimental platform for Swedish battery and steel industries

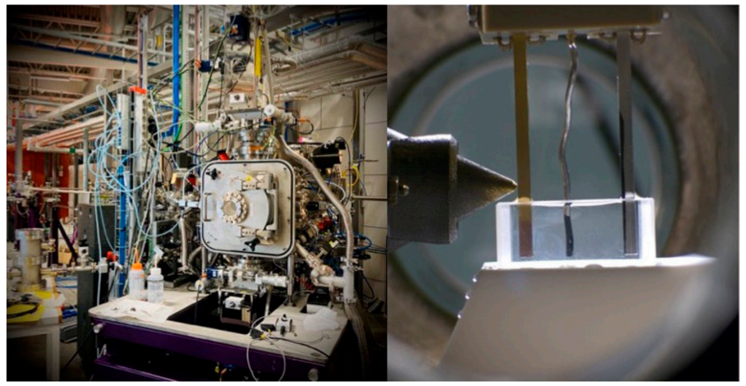


Figure 1: *Left: Solid-Liquid endstation. Right: The three-electrode electrochemical setup of the dip-and-pull experiment. On the left, a conical entrance of the APXPS Electron Energy Analyzer, pointing toward the working electrode.*

The Swedish battery and steel industries play a crucial and significant role in Sweden's economic prosperity. Both industries are world-leading producers of advanced materials such as tools, high-speed, and high-strength steels, and lithium, sodium, and metal-air/sulphur batteries. They have developed comprehensive research and development programs to support innovation efforts, a requirement to remain internationally competitive and quickly respond to today's most relevant challenges. Additionally, they consistently seek collaboration with universities, research centres, and research infrastructures, which have unique knowledge, experience, and hardware unavailable within the industries.

A critical technological challenge for both industries is designing and controlling the interfaces between solids (e.g. metallic alloys or battery electrodes) and liquids (e.g. water/gas or electrolyte solutions). Electrochemical processes at these boundaries will, for example, define the rate and direction of corrosion in alloy steels, the rate of battery charging and capacity, failure conditions in mechanical components, and the lifetime of an energy storage device. Electrochemical processes involve both charge and mass transport across the solid/liquid interfaces, and therefore require special analytical tools that satisfy several needs – namely, to be chemically specific, surface/interface sensitive, quantitative, capable of measurements under real conditions, and available for immediate and mass use.

Ambient pressure X-ray photoelectron spectroscopy (APXPS) conducted at HIPPIE beamline for academic users is among the best tools to address these challenges. However, the high demand for beamtime by multiple research communities contributes to a lack of access for industrially relevant experiments.

To address this issue, MAX IV proposed expanding the beamline's capabilities by building a new permanent endstation at HIPPIE dedicated to corrosion, batteries, and electrochemistry research with a primary focus on industrial applications. The proposal was supported by SWERIM and Uppsala University academic partners and SSAB, VBN Components AB, Gränges R&I, Alleima (former Sandvik Materials and Technologies), Ovaco Sweden AB, and battery industries via Batteries Sweden centre (BASE).

The Accessibility to Infrastructure grant 2020-06170 totalling 7.750 MSEK was provided by the Swedish Research Council. The project initiated in early 2021, and the endstation's capabilities were offered to MAX IV user communities in the autumn of 2023. Today the new endstation runs more than 50% of the activities at HIPPIE beamline.

The endstation occupies a new branchline of HIPPIE beamline and can receive light from the other branchline within minutes. The so-named B-branchline has an optical design optimised to maximise the photon flux (>1012 ph/s) at the high end of the energy range (260 eV – 2400 eV), which is beneficial for studying solid-liquid interfaces of electrochemical systems by APXPS.

The key part of the infrastructure is the electrochemical cell (figure 1, left), the sample environment where in situ and operando APXPS studies at the solid-liquid electrochemical interfaces are conducted. The primary technique available at the endstation is the dip-and-pull method (figure 1, right) where, inside the experimental chamber, electrodes can be dipped into liquid and pulled out to form a thin meniscus. The top of this meniscus is thin enough to probe using APXPS, enabling measurements of the underlying electrode surface. An argon-filled glove box can be attached to the cell, making it possible to study air and moisture-sensitive materials, such as lithium-containing battery electrodes.

USER STORY

Studying operational Li-ion battery solid-liquid interfaces

A critical contribution of academic research to battery technology development is using advanced characterisation methods to address fundamental questions of battery interfaces functionality. During HIPPIE's first commissioning experiment, an Uppsala University research group (PI Maria Hahlin) utilised the dip-and-pull method to measure the functional interface between a lithium cobalt oxide (LCO) electrode and lithium perchlorate electrolyte dissolved in propylene carbonate. Figure 2 shows the different sample positions measured differing ratios of electrolyte solution and underlying electrode surface. This measurement was done fully operando with a voltage applied to the cell, enabling the study of lithiation and delithiation reactions at the electrode surface.

The importance of this interface in batteries cannot be understated. It is here where many critical chemical processes occur, including the formation of solid-electrolyte interphases (SEI), the growth and stability of which is critical to the battery long-term performance.

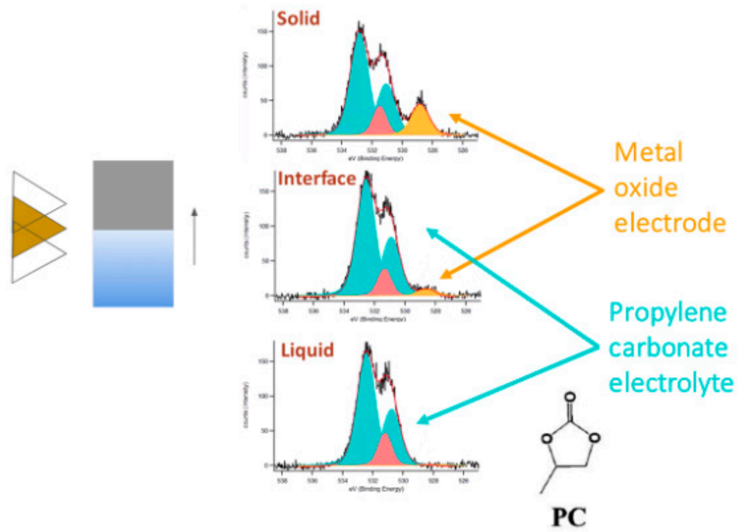


Figure 2: *Observation of the solid-electrolyte interface on an operational battery electrode under lithiation potential. (Left) scheme of the dip-and-pull measurement. (Right) O 1s spectra measured at three different points indicated on the left panel. The metal oxide electrode signal indicates the interface presence.*

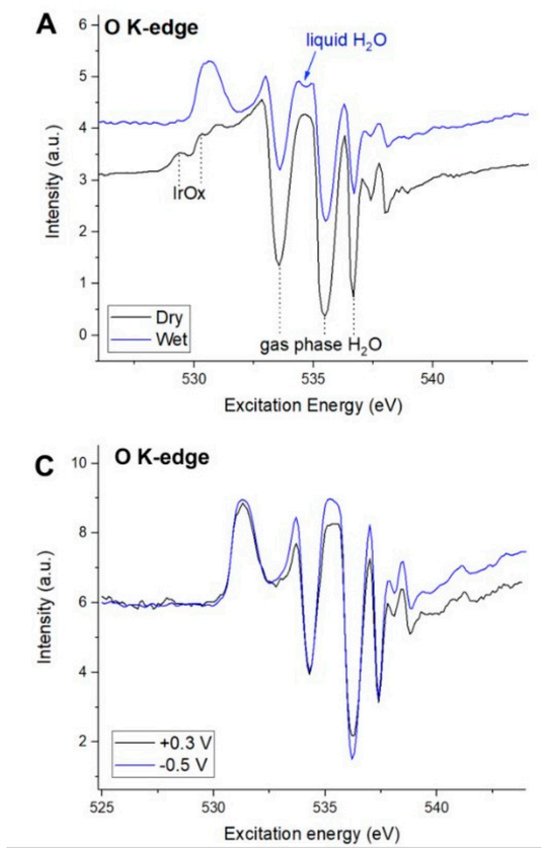


Figure 3: *O K-edge TEY-XAS spectra of IrOx under in situ (top) and operando (bottom) electrochemical conditions.*

USER STORY

Developing surface sensitive X-ray absorption spectroscopy for electrochemical interfaces

The capability to study electrocatalytic reactions occurring at solid-liquid interfaces under electrochemical control is paramount to the science case of HIPPIE beamline. A complementary surface sensitive method to XPS is total electron yield X-ray absorption spectroscopy (TEY-XAS), which measures the current of photoelectrons leaving the sample as a function of incident photon energy. This well-established method is very challenging to apply to operando electrochemistry experiments as the TEY-XAS signal is vanishingly small compared to the electrochemical currents.

A collaboration between Leiden University (PI Rik Mom) and the HIPPIE team has led to the implementation of a chopped X-ray beam synchronised with a lock-in amplifier to separate the TEY-XAS signal from the electrochemical currents. In figure 3, (e.g. O K-edge TEY-XAS) measurements demonstrate this ability in a dip-and-pull experiment of an iridium oxide electrode in an aqueous electrolyte solution.

TEY-XAS is a promising method that HIPPIE will soon offer users, as such XAS can elucidate critical chemical information not always trivial to determine with XPS alone, for example, the precise oxidation state of transition metals which underpin many electrochemical reactions.

USER STORY

Dissolution mechanism of passive film on stainless steel

Understanding the mechanisms of passive film dissolution for low and high-alloyed steels is key for the development of affordable corrosion-resistant alloys with low chromium concentrations. The in situ APXPS capabilities of the endstation were recently used by SWERIM user group (PI Konstantin Simonov) to study the dissolution process of the protective oxide on Hybrid 60 steel produced by Ovaco AB and a reference 420 stainless steel.

The samples were immersed in NaCl solution and held at various potentials. After pulling them back, photoemission spectra were measured without exposing samples to the atmosphere.

The AP-XPS results demonstrate a rapid increase in oxide thickness, increased Cr hydroxide fraction in the top oxyhydroxide layer, and decreased Cr2O3 fraction in the oxide layer above the corrosion potential onset (above +0.4 V). Further oxidation (+0.9 V) leads to the growth of Fe oxide and Cr hydroxide corrosion products and the formation of Cr6+, which can be dissolved in electrolyte and re-deposited on the sample surface.

This type of analysis was possible for the first time with the electrochemical setup of HIPPIE beamline, and now available for industrial applications.

The analysis was possible for the first time with the electrochemical setup of HIPPIE beamline and is now available for industrial applications.

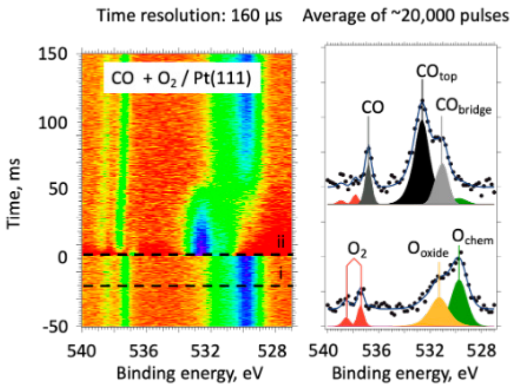


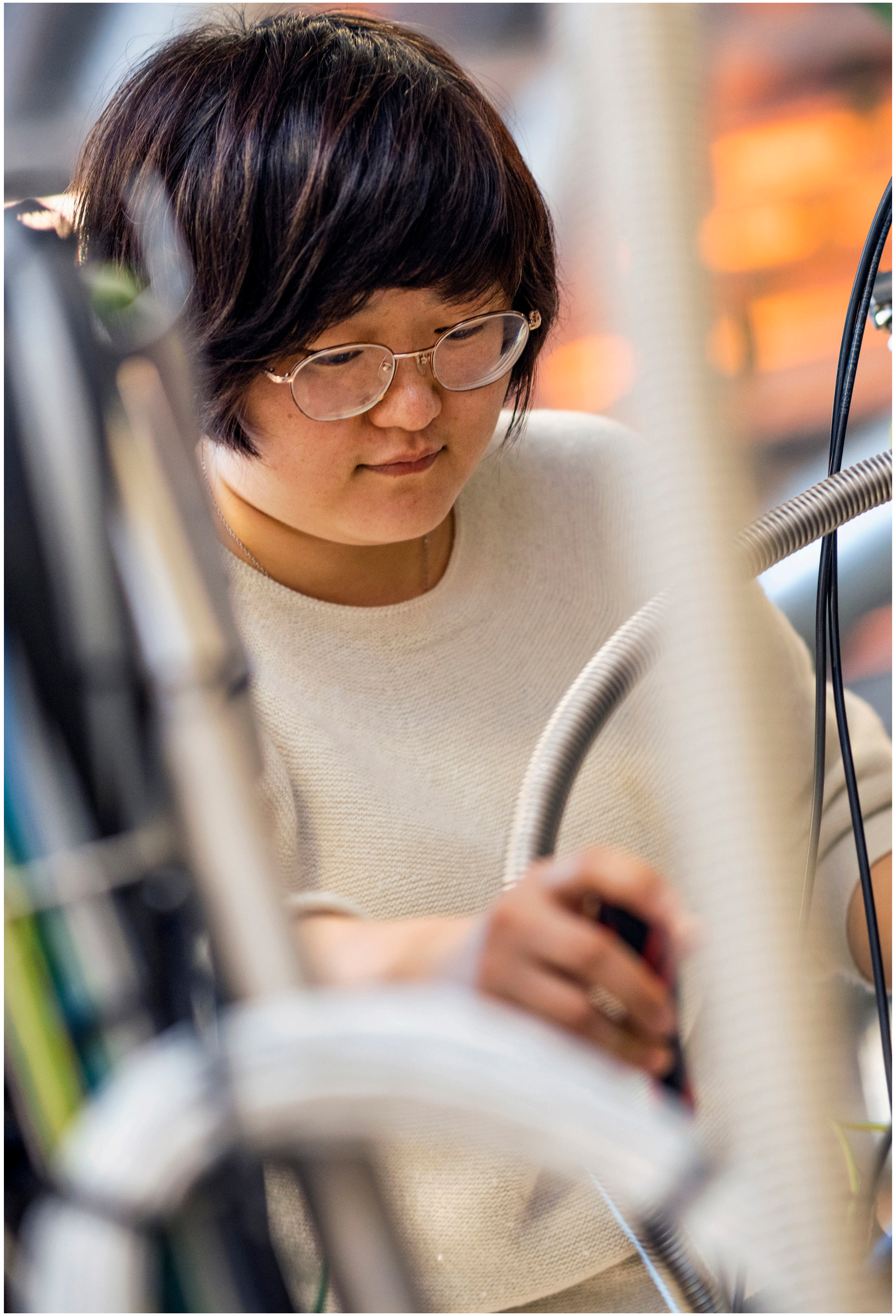
Figure 4: *Time-resolved APXPS with chemical perturbation. (Left) O1s time map of Pt(111) model catalyst measured during pulsing carbon monoxide into constant flow of oxygen gas at ca 1 mbar total pressure. (Right) example spectra measured with 160 µs acquisition time at 20 ms before and near the CO pulse.*

USER STORY: Time resolved thermal catalysis

For continuous development of APXPS instrumentation, one project objective was to equip the electron energy analyzer with a time-sensitive detector. This allows for unprecedented time resolution in time-resolved APXPS measurements with chemical perturbations. The method was pioneered at HIPPIE in collaboration with Lund University (PI Jan Knudsen) and developed for studying mechanisms of catalytic reactions with microsecond time resolution. A delayline detector is required to reach such time scales without efficiency loss (e.g. for a typical pump-probe experiment). Figure 4 left shows a time-resolved O1s spectrum of Pt(111) model catalyst exposed to a few mbar pressure of constant oxygen gas flow intermittently joined by short pulses of carbon monoxide with approximately 1 mbar pressure.

Due to the periodicity of CO pulses, time-resolved data from multiple pulses could be averaged, resulting in an improved signal-to-noise ratio for spectra measured with a very small acquisition time. The right panel of figure 4 clearly shows the quality of the averaged (+20,000 pulses) spectra measured with 160 µs acquisition time is reasonable for quantitative analysis.

The power of the method is the capability to obtain the correlation of the surface composition of the active catalyst and its reactivity. The former is seen in figure 4 as a switch from O-covered surface (-50 – 0 ms) to a CO-covered surface (0 – 50 ms) and back to O-covered surface (50 – 150 ms) between two CO pulses. The latter can be obtained in a similar manner by time-resolved measurements of gas composition above the active surface. This is the first time a structure-activity relationship was obtained on an operational catalyst with this high time resolution and at ambient conditions.



ACCELERATOR HIGHLIGHTS

FOREWORD

It has been an outstanding year for the MAX IV accelerators in many aspects. Accelerator Operations have fully recovered from the impact of the COVID-19 pandemic, bringing the number of hours delivered back to pre-pandemic levels. At the same time, accelerator uptime remained at world-class levels, mean time between failures in the storage rings continued to improve while the delivered light intensity increased in both MAX IV storage rings.

In parallel with excellent operations quality and reliability, the performance of the accelerators has further improved with a number of highlights. For the linear accelerator, these include the installation and start of commissioning of a transverse deflecting cavity system allowing studies and optimisation of our bunch compressor characteristics. These are crucial for delivery to time-resolved experiments at FemtoMAX.

In the 1.5 GeV ring, work focussed on further developing various timing modes, of particular interest to the community currently using single-bunch mode. One of the possible schemes (transverse resonance island buckets – TRIBs) was extensively tested with beamlines and further tests are planned for 2024. In addition, the commissioning of a new multiple injection kicker (MIK) provided a welcome reduction of perturbations to the stored beam at top-ups and significantly relaxed constraints on the allowed insertion device gaps and phases. The MIK development for the small ring was made possible by the previously successful installation and commissioning of a similar device in the 3 GeV ring in collaboration with the SOLEIL synchrotron in France.

The outstanding emittance of the 3 GeV ring enabled studies of fundamental aspects of the emission and focussing of synchrotron radiation, which will be relevant for present and future generations of storage ring-based sources. Additionally, a novel injection scheme was experimentally demonstrated showing that a combination of a conventional dipole kicker and a multipole injection kicker can be used to reduce the aperture requirements for efficient injection, which will be a critical requirement in future ultralow emittance rings with small dynamic apertures.

Finally, the MAX IV Accelerator Roadmap was updated following the publication of the MAX IV 2023-2032 Strategic Plan at the beginning of 2023. The updated Roadmap describes development plans for all three accelerators at MAX IV aiming to better serve its user community: from timing modes and extension of the spectral coverage down to the infrared region in the 1.5 GeV ring, through ultrashort bunches and free-electron laser developments in the linear accelerator to ultralow emittance upgrades of the 3 GeV ring. This last point, in particular, went through a major revision in 2023, which set the stage for a science-driven effort to boost the 3 GeV ring performance and sustain the competitiveness of its beamlines beyond 2030. The new MAX 4^{U} project aims to reduce the 3 GeV ring emittance to below 100 pm rad. A conceptual design study will be initiated in 2024.

ACCELERATOR OPERATIONS

The accelerator uptime statistics in 2023 (Table 1) show significant over delivery of the goals of 97% for the rings and 95% for the Short Pulse Facility. Figure 1 illustrates the performance of the accelerators in an alternative way, with uptime data on a weekly basis.

DELIVERY STATISTICS 2023

	Planned delivery	Uptime	MTTR	MTBF
3.0 GeV Ring	4776 Hours	98.1%	1.5 Hours	75.8 Hours
1.5 GeV Ring	5064 Hours	98.7%	1.4 Hours	105.5 Hours
Short Pulse Facility	4488 Hours	96.5%	0.4 Hours	10.0 Hours

Table 1: *Delivery Statistics in 2023. MTTR = Mean Time To Recover. MTBF = Mean Time Between Failures.*

Of particular note is the large drop in uptime for all three accelerators for a single week at the end of March. This was due to a single event whereby the electrical supply to the entire facility was cut for a matter of seconds. Despite this break being so short, the accelerators are heavily dependent on a stable electrical supply, and so stopped delivering. Recovery from this event took multiple hours per accelerator. Stability of delivery is one of our main goals, and so-called "perfect weeks" are a mark of our success. These are delivery weeks when the delivery of beam to users was not interrupted at all. During 2023, we delivered six such weeks to the 3.0 GeV ring, and twelve to the 1.5 GeV ring.

ACCELERATOR UPTIME 2023

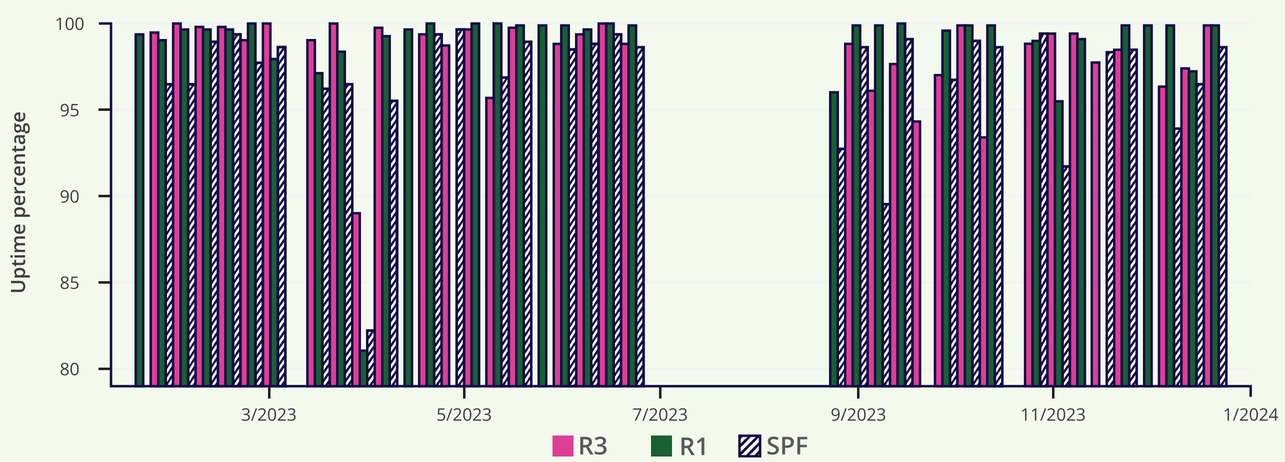


Figure 1: *Uptime of the three accelerators in 2023.*

The total integrated time that we have delivered to users has evolved considerably over the years since regular delivery started in 2017 (Figure 2). We note that we reached the international standard of around 4500-5000 hours per year in 2020 and that we have now completely recovered from the hit caused by restrictions related to COVID-19 in 2021.

Figure 3 shows the evolution over the years of the Mean Time Between Failures (MTBF). This shows that the Short Pulse Facility tends to have a failure rate of roughly twice per day, which is very good for a pulsed accelerator. The rings show strong year-on-year improvements, implying that our continuous efforts to improve operational stability are bearing fruit.

In 2023, the stored beam current (and light intensity) during delivery was raised in both rings (Figure 4). In January, the current in the 1.5 GeV ring went from 400 mA to 500 mA and in May the current in the 3 GeV ring went from 300 mA to 400 mA. In both cases, the increase is the result of a joint effort of the accelerator and engineering teams in making sure all accelerator subsystems could handle the increased current and the beamline teams that had to find ways to deal with the increased heat load on the beamline optics.

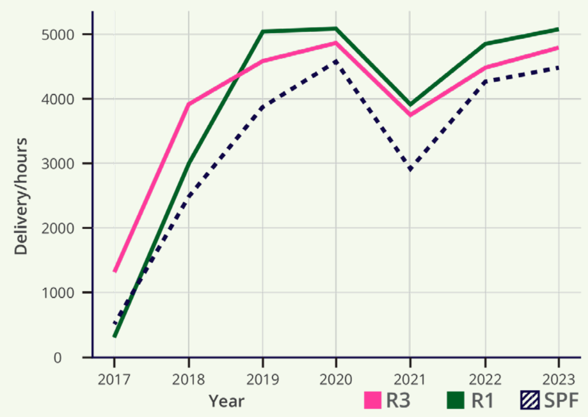


Figure 2: *Evolution of beam delivery hours since 2017.*

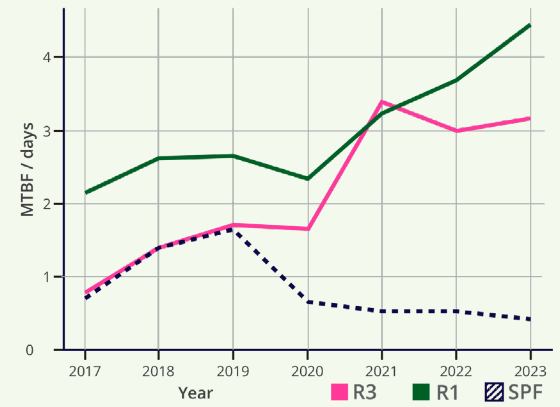


Figure 3: *Evolution of the mean time between failures since 2017.*

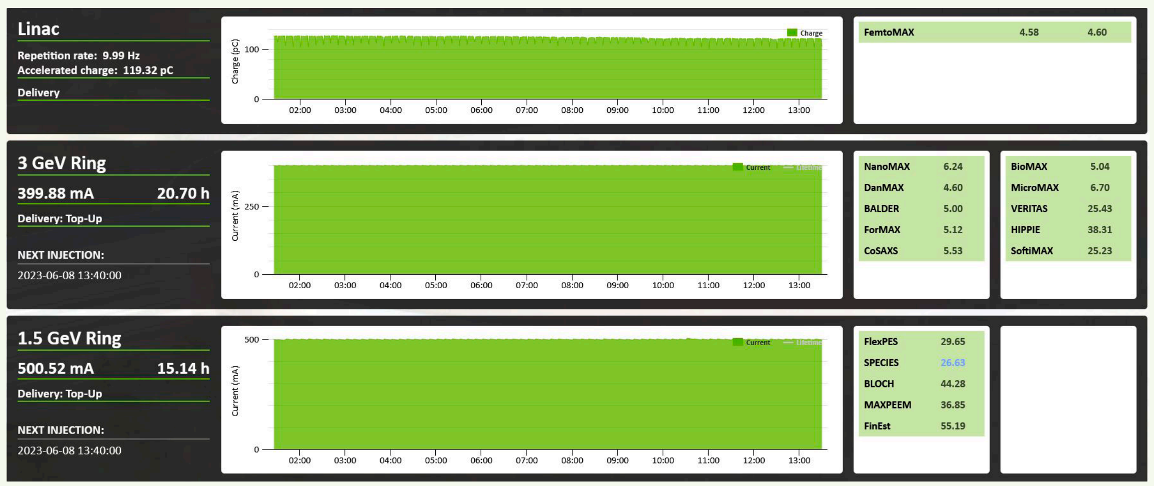


Figure 4: *Status snapshot of the accelerators in June 2023 showing 16 beamlines taking light and the increased stored currents in both storage rings.*

Compression and linearisation in double achromatic arcs

The MAX IV linear accelerator (linac) is not only used to inject electrons into the two storage rings, but also drives the Short Pulse Facility (SPF). The linac is fully prepared to handle the high demands of a free electron laser (FEL) such as the SXL.

High quality, ultrashort pulses in the range of 100 fs are delivered to the SPF. To achieve very short pulses, electron bunches are time-compressed in two bunch compressors. Globally unique, the MAX IV bunch compressors consist of achromatic arcs instead of the commonly used chicane. This allows compression to very short bunch lengths without need for a costly harmonic cavity for linearisation of longitudinal phase space. Instead, a sextupole magnet inside the compressors is utilised to adjust the longitudinal energy curvature of the electron bunch.

For delivery to the SPF beamline FemtoMAX, the electron bunch is compressed to 100 fs and linearised to create a smooth and gaussian-like current profile. The compression and linearisation scheme naturally produce a sharp peak in the centre with a low charge head and tail. Simulations show potential to compress the electron bunch even to sub-fs duration.

The start-up of a new diagnostics tool, a transverse deflecting cavity system (TDC), provides in-depth insight of how the compressors perform in practice. Measurements of both bunch length and longitudinal phase space while scanning compression (Figure 1) and linearisation (Figure 2) were made and compared to simulations. Results indicate good agreement between simulations and measurements (Figure 1, Figure 2), confirming the bunch compressors perform as anticipated.

Beyond demonstrating the success of compression and linearisation, the accelerator group successfully measured very short pulses, down to 3 fs long. This was, however, not the shortest bunch possible to produce, but the shortest measurable with the status of TDC commissioning at the time. The expectation is to produce and measure pulses down to 1 fs from the MAX IV linac in the near future.

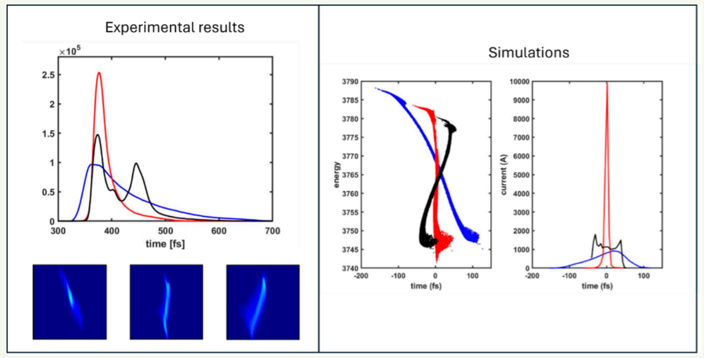


Figure 1: Experimental (left) and simulated (right) results from the TDC showing three different compression scenarios. Under-compressed (blue), over-compressed (black) and fully compressed (red). The measured electron beam corresponds very well to expectations from simulations.

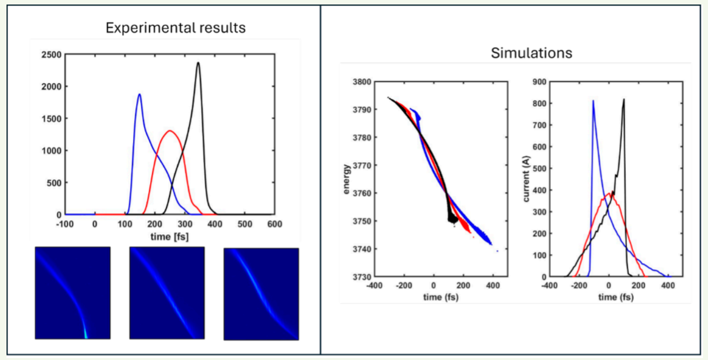


Figure 2: Scanning the sextupole magnet in the MAX IV compressors allows control of the linearisation of the electron bunch. Experimental results (left) correspond very well with simulations (right).

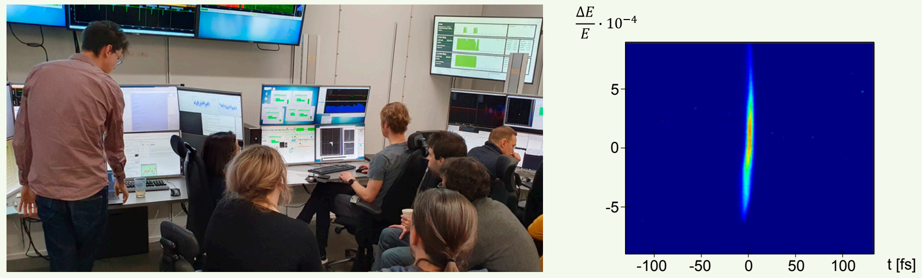


Figure 3: Scanning the sextupole magnet in the MAX IV compressors allows control of the linearisation of the electron bunch. Experimental results (left) correspond very well with simulations (right).

First beam commissioning results of the transverse deflecting cavity system

The commissioning of the TDC system began in spring, shortly after submission of the risk assessment to the Swedish Radiation Safety Authority (SSM). The radio frequency field in the TDC structures was gradually increased and, in parallel, electron beam threading and focussing were adjusted to allow for bunch length characterisation and measurements of the longitudinal phase space. Figure 3 (left image) shows the MAX IV accelerator control room when the first streaked TDC electrons were measured.

The temporal resolution of the system depends on the amplitude of the radio frequency field in the structures. The current radio frequency amplitude and electron beam parameters have allowed for 3 fs RMS measurement resolution of the electron beam. Figure 3 (right image) shows the electron beam profile observed on a fluorescent screen downstream of the TDC with radio frequency field on and a dipole spectrometer magnet active. The horizontal time axis was calculated with a measured conversion from position to time (8 mm/ps). The conversion to energy was based on the dispersion (1 m) at the location of the beam profile monitor. The longitudinal phase space, that is, energy of the electron beam as a function of time, is shown for the best resolution measurement of 2023.

Ongoing work with the TDC system aims at development of slice Twiss parameter measurements and continued efforts to bring the radio frequency amplitude up towards the design resolution of 1 fs. The TDC is an important tool for beam preparation for FemtoMAX, and an accelerator development that can enable FEL operation in a future upgrade like the Soft X-ray Laser@MAX IV (SXL).

Fast Orbit Feedback

Several upgrades were implemented on the fast orbit feedback (FOFB) systems in both MAX IV storage rings. First, the coverage was expanded. In the 1.5 GeV ring, the FlexPES horizontal plane, the last remaining uncorrected straight, was included in the global feedback loop. Following, in the 3 GeV ring, the MicroMAX insertion device straight was added, which was hitherto only stabilised using slow orbit feedback (SOFB).

Furthermore, the performance in terms of noise attenuation, specifically the frequency cut-off, was pushed above 100 Hz in both planes (Figure 4). This was the last remaining FOFB design goal, thus the system now performs according to specification.

Finally, FOFB firmware was updated in both rings based on feedback from the operations team to increase operational robustness. This includes features such as automatic cut-off for large orbit excursions, and an updated state machine.

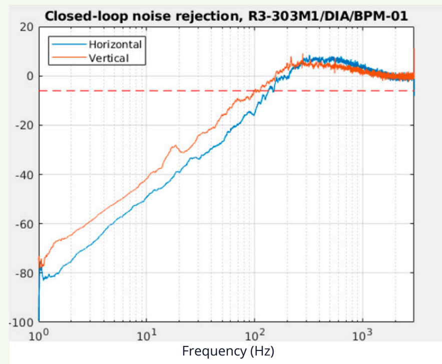


Figure 4: Measured fast orbit feedback noise attenuation for the BPM downstream of the NanoMAX ID. Note the -6 dB (half-amplitude) cut-off, which exceeds 100 Hz.

Multipole Injection Kicker (MIK) in the 1.5 GeV ring

A new injection kicker was installed in the 1.5 GeV ring at the close of 2022. It has proved extremely effective in reducing spurious oscillations on the stored beam due to the multipolar nature of its pulsed magnetic field. Early in 2023, full commissioning of the device took place, with a mechanical alignment to optimise its position with respect to the stored beam, and a tuning of the resulting injection efficiency. The operating voltage was reduced from the initial maximum value, providing more ceiling for better tuning if necessary. Measurements were taken to prove the low impact on beam disturbance during the injection process. As a final test of the MIK effectiveness, a series of measurements were performed with all beamlines in the 1.5 GeV ring, demonstrating that the MIK outperforms its predecessor (the dipole kicker, DK) in terms of injection transparency. Eloquent proof (Figure 5) is shown with an absorption spectrum taken at SPECIES while disturbing the stored beam with the MIK and the DK. Today, it is routine to operate at 500 mA, with a 10 min interval top up (previously 30min) within a wide range of ID configurations and an injection efficiency higher than 90 %.

Timing modes in the 1.5 GeV ring

Tests of transverse resonant island buckets (TRIBs) in the 1.5 GeV ring continued in 2023. This scheme, pioneered at the BESSY synchrotron, exploits the nonlinear dynamics of the machine to create a secondary orbit winding round the central 'core' beam orbit and returning on itself after three turns. This orbit thereby gives the beam three additional stable points in phase space at each location around the ring and these points are referred to as islands. The end goal is to put a single electron bunch on this secondary orbit (split between the three islands) to serve users of pulsed X-rays. Meanwhile, the usual multibunch beam would sit on the core orbit and serve users of high-intensity quasi-continuous light at the same time.

In 2023, light from this mode of operation was used by all beamlines on the 1.5 GeV ring for the first time. External users were also involved in testing the use of TRIBs light with their experiments designed for the single-bunch delivery immediately prior. This was all made possible by continuous development of the scheme in close contact with the beamlines, including a half-day internal workshop in June dedicated to timing modes on the 1.5 GeV ring. Developments included storing additional charge to the TRIBs bunch to address intensity concerns. Another important factor has been improvements to the compensation of the beamline insertion devices to maintain the sensitive nonlinear dynamics for variable photon energies. A remaining major challenge going forward in TRIBs optics will be accommodating the full range of insertion-device movement that is permitted to the beamlines during normal operation.

Work planned for 2024 includes a test of TRIBs that runs over several days so the beamlines can comprehensively characterise the light they receive, while on the accelerator side, the specific operational challenges can be identified and addressed.

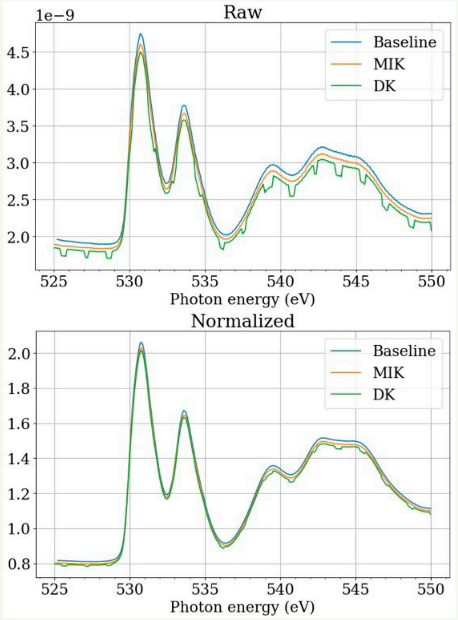


Figure 5: Oxygen K-edge absorption spectrum on a TiO2 sample as measured at SPECIES beamline. Normalisation of the signal is not sufficient to smoothen the curve when operating the dipole kicker.

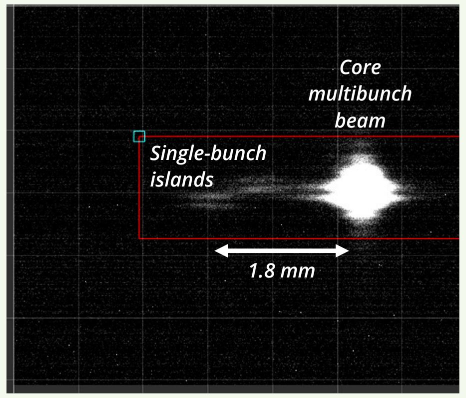


Figure 6: Transverse resonant island buckets in the 1.5 GeV ring. Only one of the 32 bunches in the ring has the islands filled whereas all other bunches follow the core orbit.

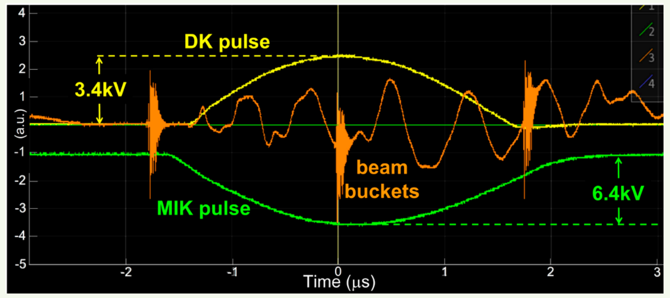


Figure 7: Oscilloscope traces of the current pulses in the dipole kicker (DK) and multipole injection kicker (MIK) used in the tandem injection scheme.

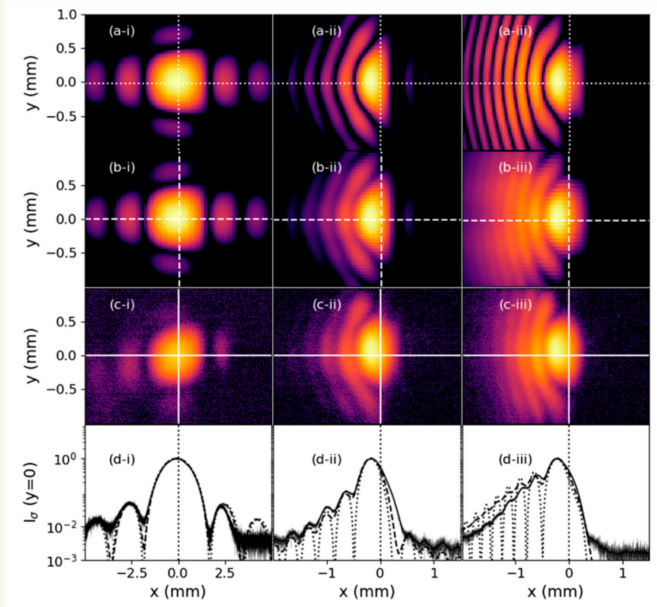


Figure 8: Theoretical 2D image intensity distributions for zero-emittance electron beam (top), for 336 pmrad horizontal emittance beam (middle), and an actual measured beam at MAX IV (bottom). The columns depict (from left to right) the case of 1.6 mrad, 9 mrad and 15 mrad horizontal collection angle.
Credit: *M. Labat et al. Bending Magnet Synchrotron Radiation Imaging with Large Orbital Collection Angles. Physical Review Letters 131, 185001 (2023).*

Tandem injection scheme reduces aperture requirement

A common challenge when injecting into ultra-low emittance storage rings is that the aperture into which the beam can be stably captured (the so-called dynamic aperture of the ring) tends to be smaller as the focussing is made stronger to bring the electron emittance down and consequently increase the photon beam brightness and coherence. While working on possible future improvements for the MAX IV 3 GeV ring, a novel injection scheme was experimentally demonstrated, which significantly reduces the aperture requirements. In this scheme, two pulsed magnets are used in conjunction – a dipole kicker reduces the oscillation amplitude of the injected beam and a multipole injection kicker about 20 metres downstream brings the oscillations of the stored beam down while almost not disturbing the injected beam. The final result is the maximum oscillation amplitudes of both beams are significantly reduced. Such a scheme could potentially be used in the MAX 4^{U} upgrade.

Synchrotron radiation emission and focussing

Fundamental aspects of synchrotron radiation emission and focussing were investigated at one of the MAX IV 3 GeV ring diagnostic beamlines. The investigation, a first of its kind, revealed intricate features of the image plane intensity distribution, not observed earlier. The observations covered the visible and infrared spectrum of the synchrotron radiation. Measurements (Figure 8) were possible owing to large angle acceptance of the bending magnet produced synchrotron radiation and excellent optic quality, ensuring clear visibility of the intricate synchrotron radiation features. The near to ideal imaged synchrotron radiation revealed an asymmetric fringe pattern, with a visibility suitable to determine a horizontal beam size of approximately 25 µm. The ultralow emittance of the MAX IV 3 GeV ring was essential to make these measurements possible (see credit in Figure 8).

The astonishing outcome of this verification of the asymmetric fringe pattern is the resolution capability increases with diminishing horizontal beam size. Thus, for small horizontal beam sizes at future ultralow emittance synchrotron radiation sources, the resolution capability will increase all the way down to approximately 5 µm horizontal beam size, corresponding for most multibend magnetic lattices to emittances below 50 pmrad. Hence, with this method, all upgraded synchro-

ACCELERATOR HIGHLIGHTS

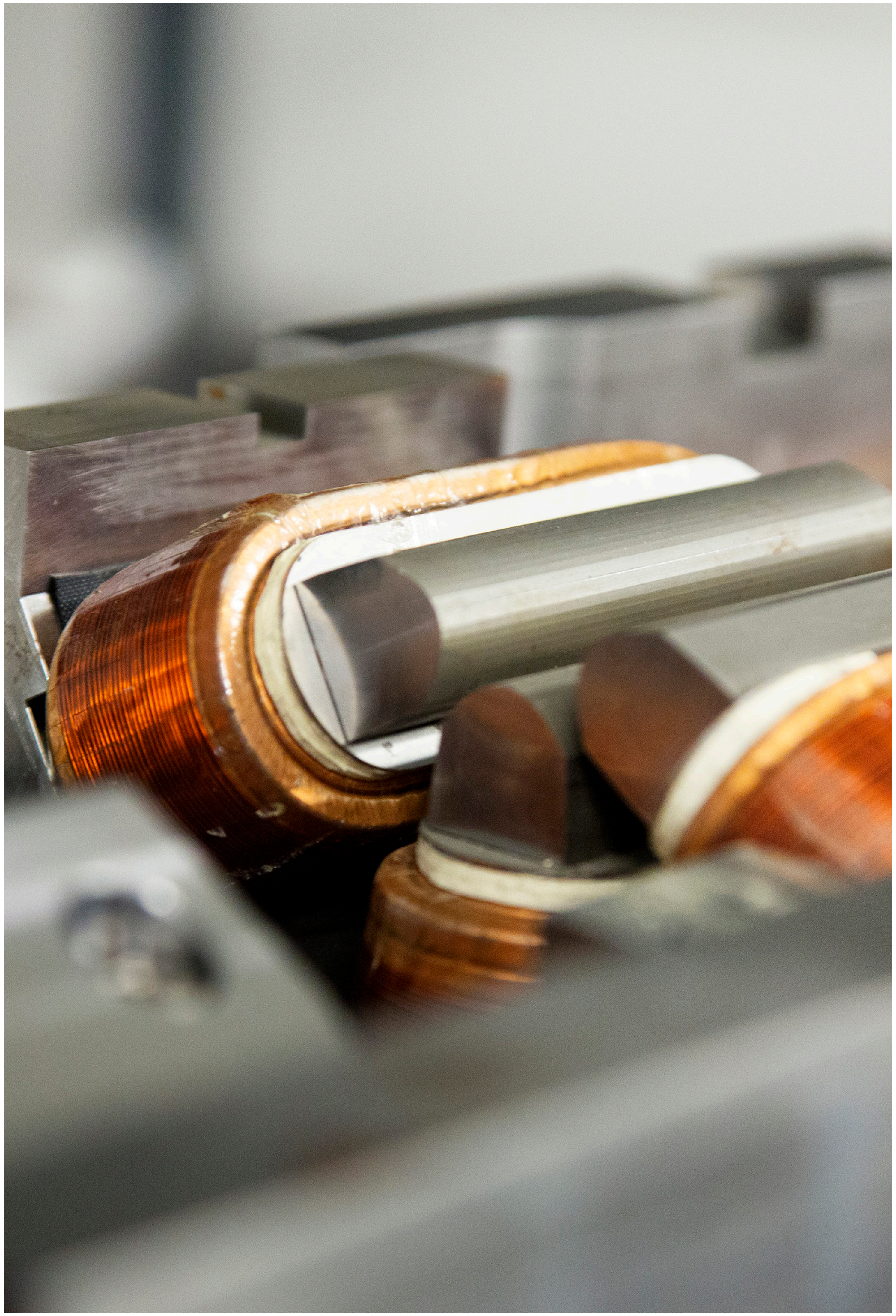
Participants of the third International Pulsed High Power Radio Frequency Sources Workshop 2023 in the MAX IV experimental hall.

tron radiation facilities have a good opportunity to measure their aimed horizontal emittance. Another fundamental aspect of focussed synchrotron radiation of wide horizontal collection angle is the intensity distribution in the image plane can be shown to asymptotically become independent of the horizontal collection angle, if it is larger than a few times the intrinsic synchrotron radiation opening angle. At MAX IV, it is roughly at larger angles than 15 mrad. This fact was demonstrated both experimentally and analytically, even though counter-intuitive (the horizontal fan of synchrotron radiation is as wide as the bending angle of the magnet). Additionally, it shows the large horizontal collection angle necessary to aim for, when performing this kind of high resolution diagnostics, is still quite accessible.

The third International Pulsed High Power Radio Frequency Sources Workshop 2023

September 18-20, MAX IV hosted the third International Pulsed High Power Radio Frequency Sources Workshop. The workshop scope was to gather experiences from laboratories worldwide on the reliability and performance of pulsed high power radio frequency systems and on future requirements regarding klystrons, modulators and radio frequency components, at all common frequency bands of L, S, C and X. The aim was to share details of good and bad experiences and all the challenging issues faced at each facility, to gain advice, recommendations and share strategies for the advancements of our institutes and coordination of development activities, where possible.

This highly successful workshop had 28 participants, representing 14 laboratories from three continents (Europe, America, and Asia). Conclusions from the workshop were very positive and all participants agreed upon continuing this workshop series. A joint development project with the goal to provide a common pulsed radio frequency diagnostics tool for all labs was established during the workshop, with active developers from several participating laboratories signing up to contribute. With this common diagnostic tool, it will be easier to compare key performance metrics between laboratories.



TECHNOLOGICAL DEVELOPMENT AND OPERATIONS

FOREWORD

The newly formed Technical Division focused its efforts on two development paths for technology and systems that will be pursued in the upcoming years. One aims to enable world-leading technology and science, while the other aims to enable operational excellence.

In spring 2023, several key initiatives for change were started. They are progressing well and will continue in 2024. One example is the Experimental Control System Reliability project and the use of TRL (Technology Readiness Level) as a tool for understanding when new functionalities are in operation steady state. The first step of the project focused on the four beamlines Balder, NanoMAX, Veritas, and Bloch, and received positive response from beamline staff. Another example is a project launched to support a shift in maintenance management from predominantly reactive to more proactive and systematic. It included establishing a Computerised Maintenance Management System as the master source of information for the MAX IV asset portfolio. Furthermore, the instalment of an IT Council was initiated to bring together the perspectives of groups ranging from system users to technical IT experts to get a more holistic view. The council will complement steering groups and the line organisation in matters related to decisions on IT system solutions with significant impact.

Collaboration with ESS also gradually increased in 2023. For instance, software groups at MAX IV and ESS organised joint workshops to exhange experience and knowledge.

As a part of the MAX IV budget process, the Technical Division implemented a new concept of using “bucketing” of pooled resources. Categories for projects and activities, including technical operation support, are being defined, and allocated resources are prioritised within the respective bucket. Additionally, the governance of portfolio management for larger projects was clarified and the concept of programmes was established.

The projects and programme portfolio

Projects and programmes in the MAX IV portfolio deliver significant novel capabilities and upgrades to beamlines, accelerators, and infrastructure. Programmes are large, relatively self-contained units with investment budgets and resources allocated by the MAX IV Management. The purpose of the programmes is to achieve strategic technological and scientific goals in the MAX IV Roadmap. Deliverables are defined within the programme projects and activities. In 2023, two programmes were active: the MX Programme and the ICT Enabling programme. The first aimed to build and develop the macrocrystallography capabilities at BioMAX and MicroMAX beamlines. It was initiated in 2022 and reached a steady state during 2023. The latter is a strategic initiative started in 2023 to integrate cutting-edge information and communication technology across various scientific and operational streams. It encompasses a broad range of projects and activities where each workstream focuses on specific aspects of technological integration and innovation. More programmes for the Engineering and Accelerator areas will be launched in early 2024. Development not included in programmes, such as reorganisation activities and many of the beamline upgrades and developments, are typically achieved through stand-alone projects.

The Central Project Office (CPO) is responsible for the high-level coordination and planning of resources across the portfolio. CPO members also act as programme and project managers, employing modern programme and project management methodologies that are tailored and scaled to meet the needs of MAX IV. In 2023, project management processes including investment and resource budget forecasting and tracking, risk assessment methods, and schedule and cost contingency estimates were further developed. The project organisation now has the necessary tools to follow up on ongoing programmes and projects effectively and is prepared for future major projects, such as new beamlines or other large upgrades.

NanoMAX imaging end station

A second experimental station, the imaging station at MAX IV's hard X-ray nanoprobe NanoMAX, was completed (see next page). The instrumentation and mechanical components have been meticulously designed and integrated by the Mechanical Design Team in close collaboration with beamline staff. The end station is optimised for the highest spatial resolution. In its fully operational state it will provide an X-ray beam focused down to a 30 nm spot, aiming for a long-term goal of 10 nm. It features a three-axis piezo scanner and a rotary stage for two-dimensional and computed tomographic imaging. An X-ray fluorescence detector will acquire elemental information with extreme spatial resolution. A flight tube, similar to that at the diffraction station, houses the existing Eiger area detector. The flight tube section with the detector is designed for easy transition between the two end stations. Fiber interferometers will measure the positions of both the sample and the FZP to achieve the necessary positional accuracy. A load-lock system is installed to avoid venting of the chamber during sample transfer. Introduced in a subsequent development phase, the system will keep the sample cooled throughout the entire sample exchange process. The design of the microscope chamber and the flight tube allows for easy passage of the photon beam to the downstream diffraction station. The station operates under vacuum, and liquid nitrogen cooling will be installed and commissioned in 2024. Initial commissioning experiments were conducted in late 2023, with regular User Operations anticipated in 2024.

Decreased scan times for time-resolved experiments and mesh scans

The PandABox system developed by Quantum Detectors provides advanced synchronous triggering and data capture capabilities. With this equipment as the core of the beamline data acquisition system, the Software group implemented novel triggering schemes for time resolved experiments at the beamlines CoSAXS and FemtoMAX. At Balder, the new hardware orchestrated scanning implementation that allows seamless chaining of several techniques such as XANES, XRD and EXAFS, resulted in a decrease in average scan times by more than 50%. At ForMAX, the deadtime in continuous mesh scans was greatly decreased by avoiding to rearm the detectors at the start of each line. This was done by improving the overhead time per line in the Sardana scanning framework, to align better with the MAX IV use case.

Metadata collection and integrating pixel detectors

The metadata catalog SciCat is now integrated into all beamline control systems at MAX IV. The first publication of data through SciCat, accessible via PANOSC search tools, showcased an experiment at BioMAX demonstrating the feasibility of an integrating pixel detector (JUNGFRAU) for serial crystallography.

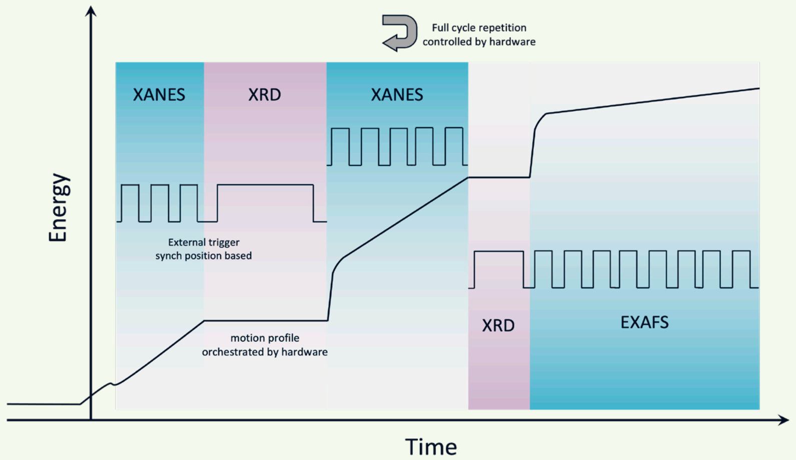
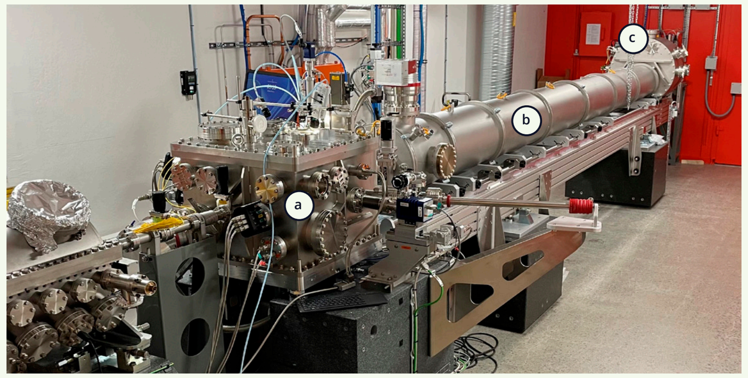
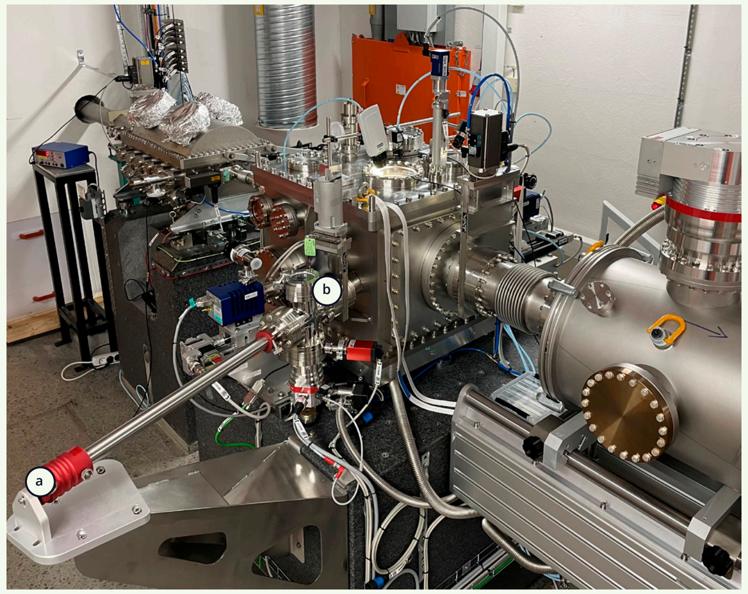


Figure 1: Balder Hardware Orchestrated Scan implemented with PandABox.

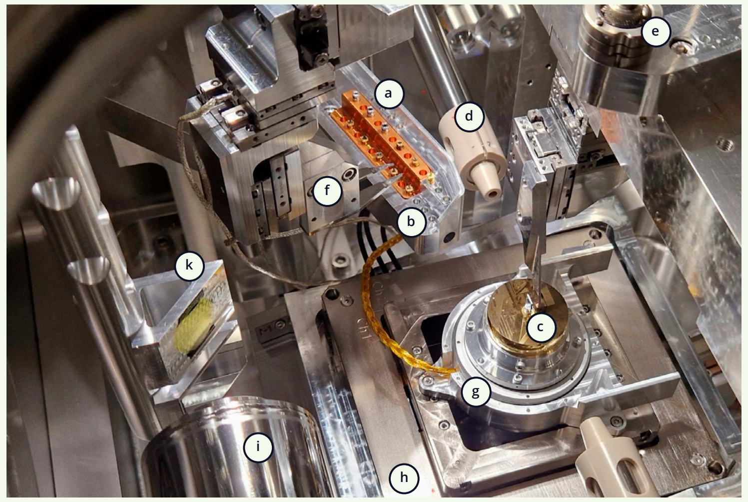
New imaging endstation in NanoMAX. Experiment chamber (a) and flight tube (b). An Eiger2X4M detector (75μm pixel size, Dectris, Switzerland) is placed inside the flight tube chamber (c).



Experiment chamber. Sample transfer arm (a) with load-lock (b).



Placement for sample tray with twenty samples mounted on OMNY pins. (a) Six spots for reference samples. (b) Measurement position. (c) Fluorescence detectors (RAYSPEC 50mm2) with collimator cones. (d) Fibre interferometer. (e) Motorised gripper arm for sample loading. (f) Rotary stage. (g) Scanner stage. (h) Optical sample microscope inside tube. (i) Mirror. (k) Fluorescence screen.



Synchronised non-linear motion trajectories

Beamline components are sometimes required to execute motions along non-trivial and non-linear paths. Therefore, a concept of trajectories has been introduced, where each motor in a system is given a unique trajectory table to follow while maintaining synchronisation. Motion trajectories are used with clear benefits in, for example, the SCANIA spectrometer at the Balder beamline, the flight tube at CoSAXS, and monochromators of FlexPES and FinEstBeAMS, as well as the Veritas Rowland spectrometer which is explained in the figures.

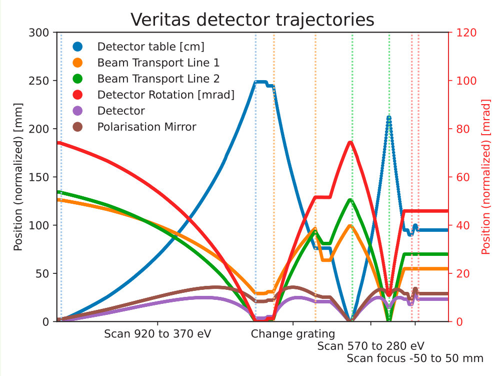


Figure 2

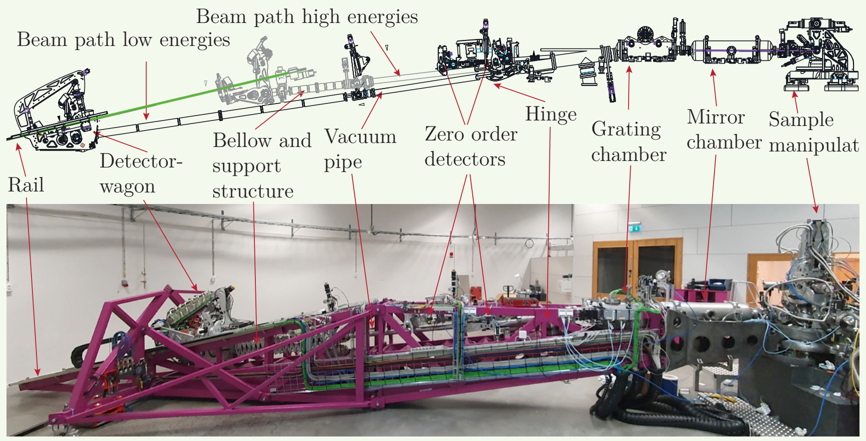


Figure 3

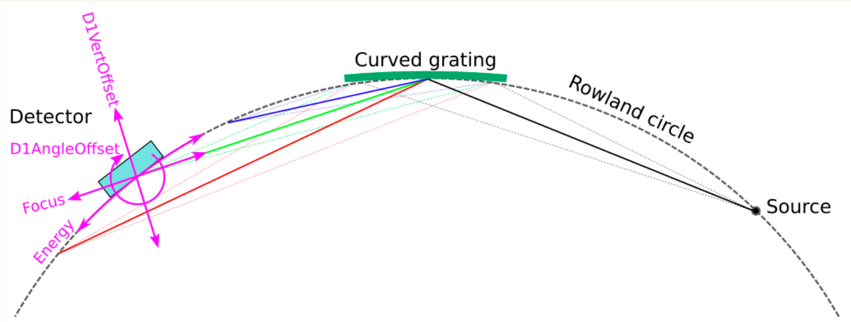


Figure 4

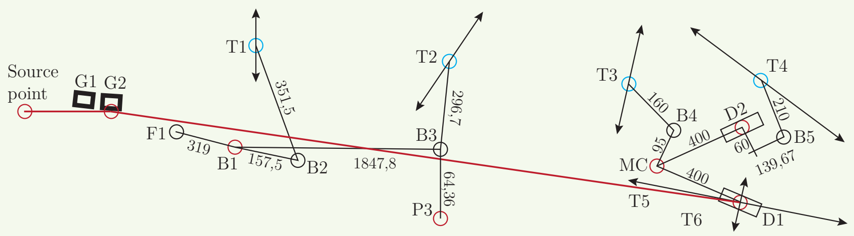


Figure 5

Figure 2–5: The Veritas 10m spectrometer arm (Figure 3) operates under the Rowland condition (Figure 4) and consists of a system of six linked axes (Figure 5) that must maintain the position of the detectors while avoiding any damage to the mechanical structure i.e. "put the red circles on the red line". The non-linear motions measured in Figure 2 are constructed as a trajectory through energy or focus space. The trajectory changes whenever any parameter changes or when moving through focus space at fixed energy instead of through energy space. Such changes result in automated generation and uploading of new trajectories.

Detector-DAQ operations and scientific software support

The Scientific Data group made significant progress in unifying the integration of the beamline end-station detectors and cameras into a common data acquisition scheme, with a focus on those systems that require high throughput online data processing and visualisation (see Figure 1). Working closely with the IT Infrastructure group, over 30 systems of ten uniquely different hardware types are now connected to a Kubernetes-managed central DAQ cluster, sharing common data processing pipeline elements to minimise the overhead in operational support. Online data processing steps common to scattering methods are now found at many beamlines developed more domain-specific pipelines, for example working closely with DanMAX and ForMAX to implement streaming tomography reconstruction. The general scientific computing support has continued in the ongoing development of the JupyterHub and HPC services and the provision of scientific software support for analysis and visualisation, ranging from XAFS experiments at Balder to RIXS at Species and Veritas.

FemtoMAX control system and time-resolved experiments

To allow the addition of new time resolved functionality and to increase the usability and reliability of the experiments, the FemtoMAX beamline control system was substantially refactored and brought into line with the standardised Sardana scanning software tools. This also allows the KITOS support organisation to begin FemtoMAX comprehensive operations support.

Unattended User Operation for MX

The MX program reached a major milestone in achieving the first collection of user data at MicroMAX beamline and substantially extending the unattended operation capabilities at BioMAX.

Data management seminars

In June 2023, the IT and Control Systems groups hosted a series of staff seminars covering scientific data management topics at MAX IV. The sessions delved into the data storage infrastructure, metadata collection with SciCat, and data analysis using JupyterHub and the high-performance compute cluster.

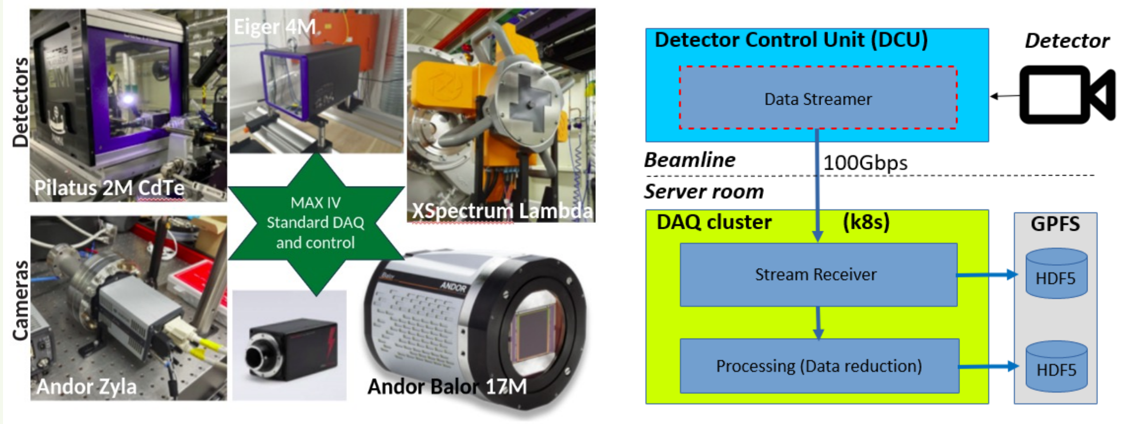


Figure 1: A wide variety of high-rate detectors and cameras (left) are now managed by a common data acquisition scheme (right) in which their data are streamed to a Kubernetes-managed central DAQ cluster for saving or further online processing.

Operation support – IT and control systems

2023 marked the second year of the KITOS operation support organisation, which provides operation support on all controls and IT related matters to the accelerators and beamlines (see Figure 2). Statistics provided by the KITOS intervention logs were used as input to the Experimental Control System Reliability project. KITOS also provided training to the Floor Coordinators and gave staff seminars on basic usage of the control system and the on-call service.

IT resource improvements

The MAX IV facility is already mature enough to go through upgrade cycles of the IT infrastructure. This is an ongoing process everywhere in IT and we just want to highlight a couple that make significant impact.

The wireless service was updated to the latest Wi-Fi technology. At the same time, we added numerous new access points at locations that were determined by a radio survey of MAX IV buildings. This enables higher transfer speed and significant improvement of coverage, especially around the experimental facilities. A portal for allowing wireless access to guests in a secure way is now also in operation.

For data collection and data analysis, incremental improvements have been made to the whole chain. On the backend, updates to storage systems and storage network have doubled the scientific storage capacity and throughput have increased by 50%. The network from detector to data acquisition (DAQ) systems can now provide bandwidth up to 100Gbit/s at all experimental areas and the available resources in the DAQ cluster have doubled. On the processing side, several new graphics accelerator (GPU) resources are available and can now be used directly from the JupyterHub service in addition to the high-performance compute HPC service.

Monitoring PLC network

The Automation team has developed an engineering GUI to monitor status and health of the PLC network system of MAX IV (see Figure 3). With this, an easy overview of the system can be used both to predict and prevent failures as well as make recovery in case of failure more effective.

Technical infrastructure upgrades

Upgrading critical central technical infrastructure is well underway. Replacing a costly, unmonitored and labour intense method of reducing oxygen content in our water systems with an automatic system based on a nitrogen generator with full PLC monitoring has successfully been carried out in W1 (linac cooling) and is ongoing for W2 (storage rings and BLs). Replacement of local, standalone constant pressure units on the water circuits (nine in total) that historically caused several beam dumps is ongoing. The new unit is developed in-house, using our central system for pressurized air, and is controlled and monitored by PLC. Planned to be finalised in 2024.

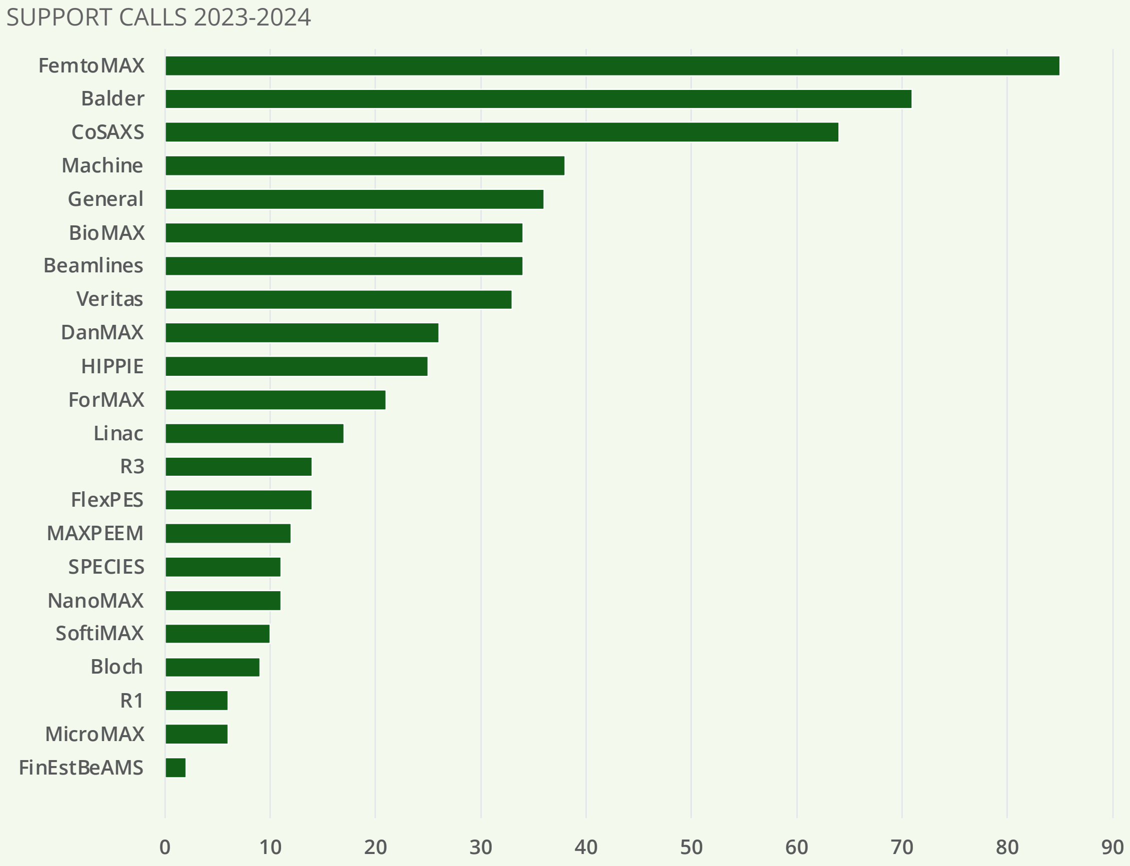


Figure 2: *Support calls per beamline during 2023–2024.*

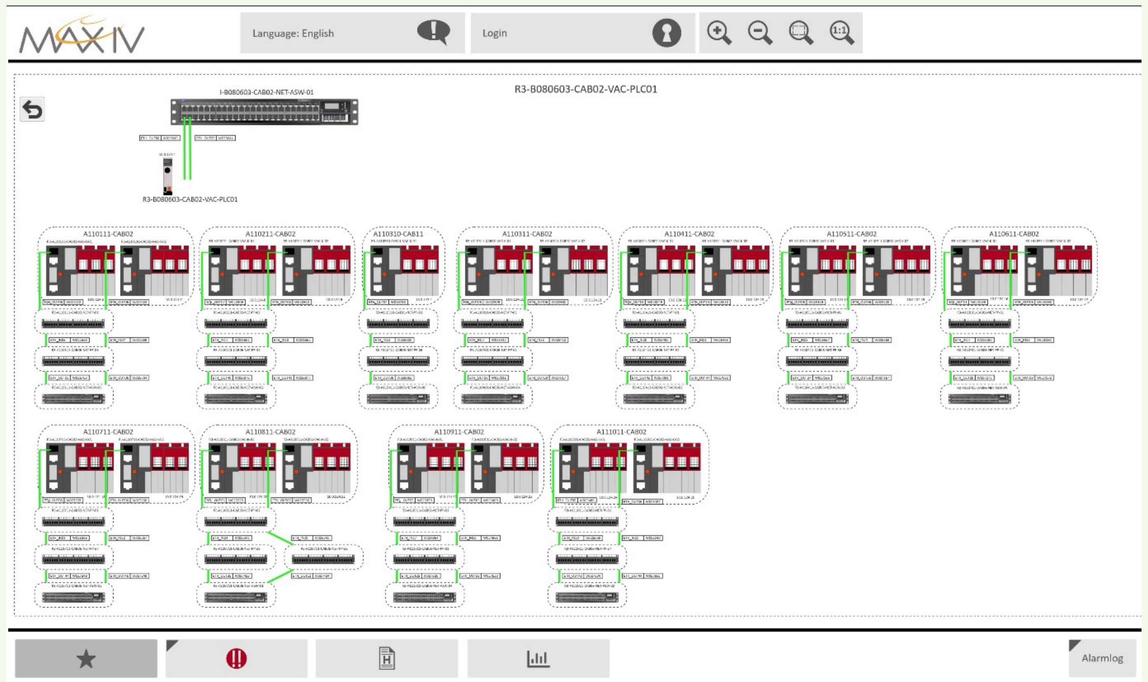


Figure 3: *Engineering GUI -example of PLC status overview.*

BUILDING INFRASTRUCTURE

The growth and expansion that MAX IV is experiencing will continue in the coming years, requiring new infrastructure solutions. In 2023, alternative and sustainable solutions for construction, logistics, and office spaces were assessed to address this need further.

The current infrastructure will not suffice to cover future extensions of the beamlines and the needs of logistics, storage, and office spaces. The main MAX IV building, for instance, lacks a separate storage warehouse, and the areas currently used for storage may be needed for the development of future beamlines. Additionally, the ventilation system, especially in the laboratory, needs improvement.

In 2023, discussions focused on how to solve these needs with local solutions. The need for more office space has been temporarily solved with the secondary satellite office space called the Cube, located close to the main facility where more employees moved in 2023. MAX IV will be a tenant of these offices up to 2027 while investigating long-term solutions. In parallell, long-term solutions and investments were investigated that could reduce the risk that comes with increased interest rates and costs for maintenance, materials, rent, electricity, cooling, and heat that will naturally increase with the growth of the facility. As MAX IV consumes a large amount of electricity, the electricity costs risk a significant increase. These discussions will continue in the following year.

Sustainable and circular efforts

With a track record of several prestigious environmental building performance rankings such as “Green Building,” “Miljöbyggnad Guld,” and “BREEAM Outstanding,” sustainability remains a guiding light for MAX IV in this work. An extensive programme for sustainable construction was implemented to attain the high environmental standard Miljöbyggnad Guld (Environmental Building level Gold). This included the installation of LED lights in all buildings, controlled ventilation, and green roofs. The latter improves insulation and helps stabilise the temperature in the experimental halls while reducing the impact on the sewage systems and improving the wildlife environment.

The ambition is to use only electricity coming from renewable sources, primarily wind and water. A modest amount of electricity will also be generated by solar panels on the roof of the office building. Additionally, dedicated efforts have been made to recycle and reuse the excess heat generated from the linac and accelerators. All accelerator equipment is connected to a cooling system with heat exchangers and heat pumps, which makes it possible to reuse the excess heat via the district heating system in Lund in exchange for cooling water for the accelerator equipment.

Leasing and contracts

MAX IV is fully responsible for the maintenance of the main building, with supplier Caverion (procured from 2021 to 2027) managing the daily maintenance and support for technical installations and upkeep, including technical and property management. The building is leased by Lund University from the owner Fastighets AB ML 4, a joint corporation between Peab Sverige AB and Wihlborgs Fastigheter AB.

COLLABORATIONS AND OUTREACH

Collaboration is a key strategy to maximise the utilisation of MAX IV and enable leading innovation and frontier science with user communities. In 2023, this was achieved through various collaborative projects, participation in networks and communities, and targeted outreach efforts.

Partnerships and collaborations

MAX IV staff proactively seek external funding to support facility development, both as lead applicants for funding and as project partners collaborating with academia and industry. In 2023, the number of individual project grant applications involving MAX IV submitted to national and international funding organisations increased by nearly 100%, from 34 in 2022 to 66 in 2023. In over a third of the cases (38%), the project's main applicant was a MAX IV staff member. The primary applications were led by external collaborators (see Figure 1a and 1b). The 66 individual project grant applications were submitted to 19 different funding agencies, most of which are based in Scandinavia (See Figure 2, next page).

As of February 2024, the success rate of the submitted applications was 32%, with 21 approved and 17 still under review. It is notable that out of 17 applications involving MAX IV submitted to the Swedish Research Council, 15 were submitted to the research project grant Röntgen-Ångström Cluster. Two were approved, with MAX IV as a project partner. Three applications were submitted to calls by Scandinavian institutions (the Academy of Finland, Carlsberg, and Novo Nordisk Foundation). Ten applications were submitted for funding from European Commission programmes, mostly from calls within Pillar 1 of Horizon Europe (Infrastructure Calls and Marie Skłodowska Curie Actions).

Among the approved applications: "Upgrade of the SPECIES ambient pressure cell", granting MAX IV a budget of 2 MSEK by the Crafoord Foundation. The proposed instrument is a multifunctional sample environment that can support fundamental and applied research in many fields of science and technology. It will be designed to mimic the conditions in many industrial processes and be especially useful for studying sustainable steel production, high-temperature corrosion, catalysis, and solid oxide fuel cells. These opportunities will attract new user communities to SPECIES beamline particularly from the steel

MAIN PROJECT APPLICANT AFFILIATION STATISTICS 2023

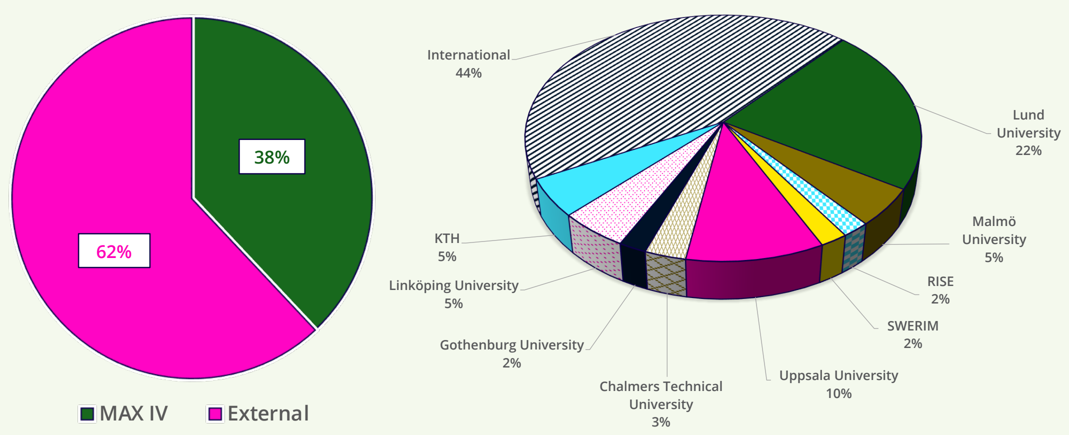


***Figure 1a (left):** Graphical distribution of the affiliation of the main applicant of project applications.*
***Figure 1b (right):** Percentage of project applications per main applicant affiliation involving MAX IV as partner.*

APPLICATIONS PER FUNDING AGENCY 2023

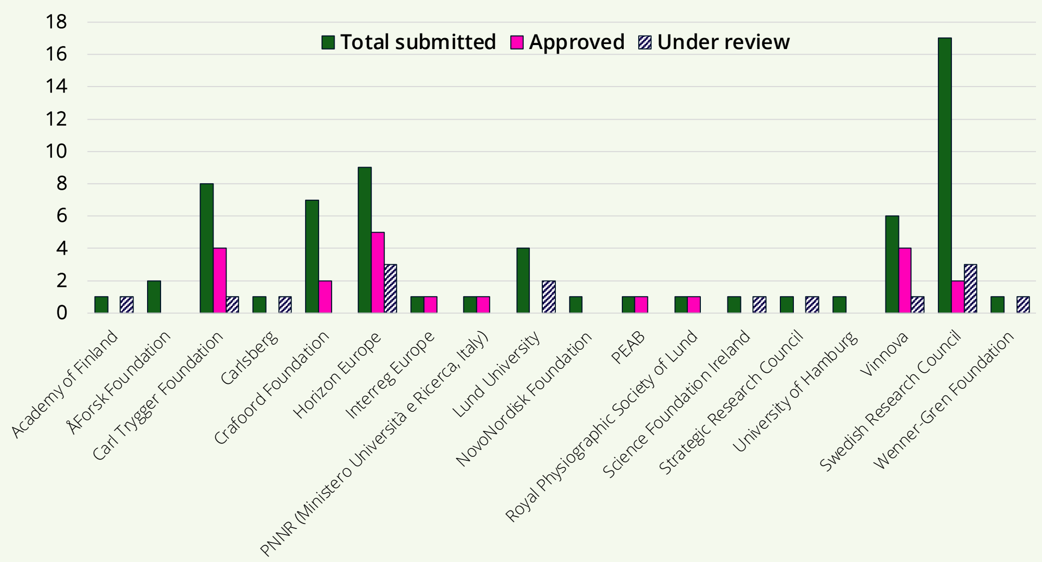


Figure 2: *Total number of applications submitted, accepted, and currently under review per funding agency in 2023 (known as of February 2024). Funders are listed alphabetically.*

industries. Additionally, the Carl Trygger Foundation approved four applications with a total budget of 1,170 MSEK promoting upgrades of CoSAXS, FinEstBeAMS, and HIPPIE beamlines and providing support for relevant conferences organised by MAX IV to encourage outreach.

The support granted by Swedish foundations through funding of external projects, aside from the contributions to the operational budget or big investments such as in new beamline construction projects, is crucial to support keeping MAX IV at the forefront of science.

Funded external research projects

In 2023, MAX IV was involved in 55 externally funded projects with funding from 18 funding agencies. The total contract amount for these projects was 225,530 MSEK (see Figure 3). MAX IV is the project lead in 22 of these external projects and received funds for 23 additional projects as a collaborator. In seven of the external projects, MAX IV's participation is In-Kind.

The PRISMAS project (PhD Research and Innovation in Synchrotron Methods and Applications in Sweden) was initiated in 2023 with funding from the European MSCA COFUND programme. PRISMAS is coordinated by MAX IV and involves eight Swedish universities. In 2023, the two first calls were successfully executed to employ a total of 40 PhD students related to five science areas. The interdisciplinary approach promotes knowledge exchange across research fields and universities in Sweden, training the next generation of synchrotron X-ray scientists and users. Several other projects reached significant milestones in 2023, such as ReMade@ARI, which completed its first call for transnational user access to a consortium of approximately 50 participating facilities. ReMade@ARI, centrally managed by MAX IV, aims to enable the development of new materials with high recyclability and competitive functionalities. It is funded by the Horizon Europe Call HORIZON-INFRA-2021-SERV-01, with a total budget of 13,7M€, coordinated by Helmholtz-Zentrum Dresden-Rossendorf research laboratory (HZDR). The project bolsters MAX IV's visibility among the international academic user community and focuses on increasing the use of research infrastructures by SMEs and other industrial users.

Seven new external projects started in 2023, some of which received a funding decision in 2022. MAX IV is the project lead for two of the seven projects. MAX IV also received funding for three additional projects as a collaborator and is involved in two more projects with no transferred funding.

CONTRACT AMOUNT (SEK) PER FUNDING AGENCY 2023

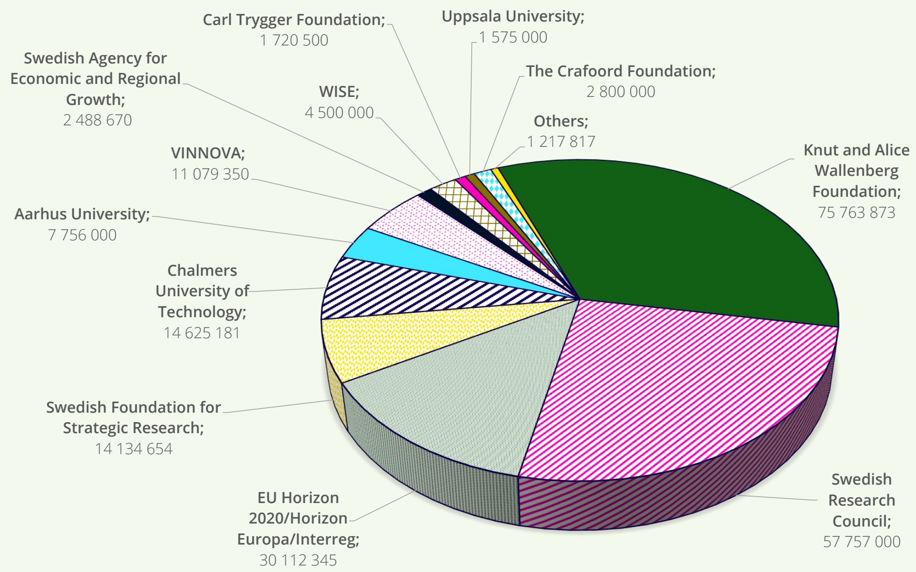


Figure 3: *Contract amount in SEK per Funding Agency in 2023 (total: 225,530,390 MSEK), excluding projects that ended in 2023. The grant values relate only to research projects and do not include funding for beamline construction projects.*

Ongoing national and international collaborations

MAX IV continues to develop collaborations with national infrastructures in Sweden, for instance, through the IntraLife and InfraVis projects. There are also ongoing dialogues with the Lund Laser Center and the European Spallation Source (ESS), and collaborations with networks such as Treesearch, Northern Lights on Food, and Metalbeams to foster strong collaborations between academia and industry. These collaborations contribute to ensuring that Swedish research remains at the scientific forefront.

As a foundational step towards the future of MAX IV, the Wallenberg Initiative Materials Science for Sustainability (WISE) granted MAX IV 4,5 MSEK to produce Conceptual Design Reports for three new beamlines enabling materials science for sustainability. These beamlines would complement the existing spectroscopy capabilities of MAX IV with hard and tender X-rays (supporting techniques such as HAXPES), diffraction with operando surface and powder X-ray diffraction at high frame rates, and full-field X-ray imaging and tomography with absorption and phase contrast. The reports were collaboratively developed through workshops with the scientific community and submitted to WISE by the end of 2023.

At the European level, MAX IV is actively involved in the League of European Accelerator-based Photon Sources (LEAPS) and has ongoing collaborations with BESSY (Germany), Synchrotron SOLEIL (France), and SOLARIS (Poland). MAX IV is also involved in Lightsources.org, and the Analytical Research Infrastructures in Europe (ARIE). These networks promote the exchange of information and knowledge, which often leads to project applications and the creation of consortia applying for EU funding. Furthermore, MAX IV's involvement in European initiatives that focus on promoting research in specific research areas include the ReMade@ARI project, which fosters the use of research infrastructure for circular materials research.

MAX IV also has collaborations beyond Europe. In April 2023, MAX IV organised a workshop on the science opportunities with diffraction-limited soft X-rays scheduled in Port Jefferson (NY, USA) with several of the lightsources funded by the United States Department of Energy. There are also ongoing collaborations with the SLAC National Accelerator Laboratory (USA).

More recently, MAX IV initiated the process of developing a collaboration with Tohoku University (Japan), which hosts the new synchrotron radiation research center Nanoterasu.

INTERNATIONAL COLLABORATIVE PROJECTS RUNNING IN 2023

A collaboration that aims to deliver standardised, interoperable, and integrated data sources and data analysis services for photon and neutron facilities.

EU-supported initiative to increase companies and hospitals engagement in research collaborations with research infrastructures in the Öresund-Kattegat-Skagerrak (ÖKS)-Hamburg area.

NFFA-Europe is a center for research infrastructure that integrates nanofoundries.

A central hub for circular economy research – network of 48 facilities supporting recyclable material science.

European hub working with long-term partnerships between industry and European light sources, synchrotrons and free-electron lasers.

The consortium enables access to structural biology research infrastructures for all European researchers, including non-experts in structural biology.

PhD Research and Innovation in Synchrotron Methods and Applications in Sweden – is a doctoral programme that trains the next generation of leading synchrotron experts.

Read more about national and international collaborative projects MAX IV is involved in via: ***maxiv.lu.se/collaboration***

Communication and outreach

With 16 funded beamlines, MAX IV has also entered a new stage of communication and outreach. This stage entails strengthening the MAX IV identity, updating the narrative, and positioning MAX IV in the research ecosystem by clarifying its role. The development of an updated five-year communication strategy for MAX IV began in 2023. It primarily aims to raise awareness of MAX IV and its scientific contributions, and strengthen the sense of community and purpose among staff. It will be implemented in 2024.

An internal communication survey and an external stakeholder analysis were conducted as part of the strategy work, involving MAX IV staff and key representatives from academia, institutes, funders, industry, and the user community. The surveys showed a need for more transparent communication and clearer reporting on finances as well as MAX IV's short-term and long-term contributions to society. To prepare for future impact reporting and communication, an internal working group was appointed to develop a KPI framework for impact measurement.

As more media exposure will follow as a result of increased press activities in the coming years, MAX IV spokespersons were identified and media trained, and a new press room webpage was created. A press release on the first-ever industry experiment at ForMAX beamline conducted by Tetra Pak, jointly distributed by MAX IV and Tetra Pak in February 2023, highlighted such a need. It resulted in various interviews and publicity in over 100 national and international news channels.

An editor was appointed to oversee and lead the alignment of MAX IV's internal communication. To keep everyone informed, weekly updates from the Senior Management Team and a monthly newsletter were distributed digitally throughout the year. Additionally, monthly staff meetings were held to encourage dialogue and celebrate achievements within the organisation.

In June 2023, the first-ever annual report on the industrial use of and collaborations with MAX IV, MAX IV and the Industry, was issued. Press efforts resulted in media coverage in many Swedish news channels. A few months later, just after the publishing of the MAX IV Highlights 2022 report, the work began with shaping the new MAX IV Annual Report you are now reading.

The Communications Group increased the use of video as a storytelling format and the focus on research news connected to sustainability as a content topic. LinkedIn was the prioritised channel as it has proven to be effective and cost-effective for engaging with the scientific community. Tactic social media efforts led to a 27% increase in followers across all channels compared to the previous year, according to the social media management tool AgoraPulse. In total, MAX IV's content on LinkedIn reached 197,500 followers in 2023, up by 21% from 2022.

SOCIAL MEDIA FOLLOWERS 2019-2023

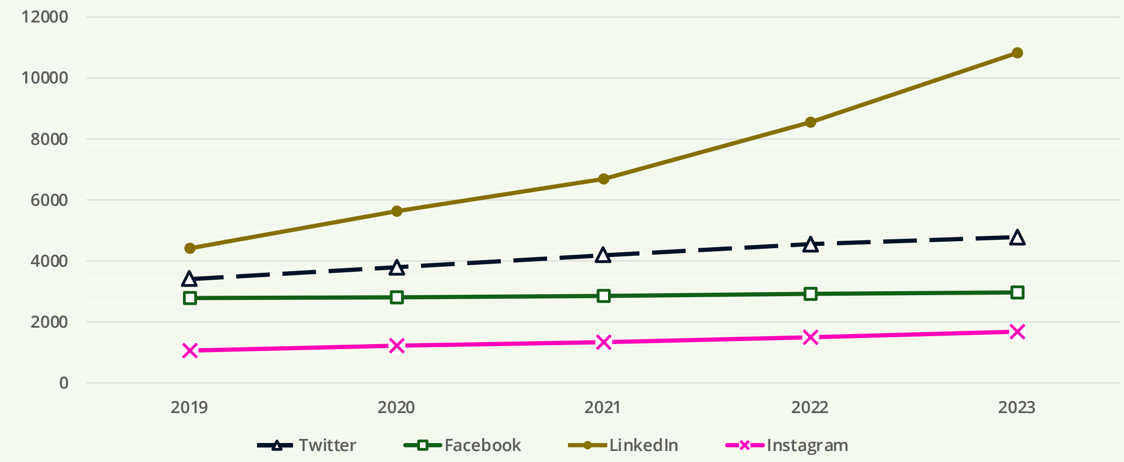


Figure 4: Number of social media followers in MAX IV's channels over the past five years.

MAX IV staff (green t-shirts) demonstrating science to visitors at the MAX IV Open day in September 2023.

Science news stories highlighting published papers and interviews with MAX IV users have been published on maxiv.se and in social media throughout 2023. The aim is to showcase the broad range of research conducted at the beamlines and inspire new user groups.

In September 2023, MAX IV organised Open Day, the first major public event in years. The event was a resounding success, attracting almost 1000 visitors and tickets sold out in record time. Many employees volunteered to help. The exhibition showcased various interactive science stations and booths, including Vattenhallen, Tetra Pak, and the Lund Robotics group with Buster, the robot dog. According to evaluation surveys, the Open Day successfully raised public awareness and understanding of MAX IV, and the interaction with scientists was highly appreciated. The event will be organised again in 2024.

As part of the collaboration with the United States Department of Energy, MAX IV organised a workshop on science opportunities with diffraction-limited soft X-rays in New York (USA) with the Advanced Light Source and National Synchrotron Light Source. The event examined new and emerging research opportunities enabled by diffraction-limited soft X-ray beams.

In June 2023, over 200 participants in the EU conference The Potential of Research Data: How Research Infrastructures Provide New Opportunities and Benefits for Society toured MAX IV. The conference was part of Sweden's Presidency of the Council of the European Union and hosted by Sweden, the Swedish Research Council VR, and Vinnova. Participants met with scientific staff and management, and the MAX IV Director gave a joint talk with the ESS Director General highlighting research opportunities in the Skåne region.

In general, the number of visitors to MAX IV significantly increased in 2023. A new Visits Policy was developed and implemented, and internal workshops were conducted to support MAX IV researchers in tour guiding and science communication. The on-site exhibits also underwent updates. Upon entering the MAX IV building, visitors now find a new exhibition in the reception area celebrating the laboratory's beginnings. It was installed in 2023 and features important milestones in MAX IV's history, including a display of the silver medal awarded to Mikael Eriksson from Lund University for his work developing the MAX IV technology. Starting in 2024, MAX IV will also be able to welcome visitors digitally through an online Virtual Reality tour developed in 2023.

Collaborative outreach efforts with ESS included a session hosted for the Teacher Education Day LU 2023, where MAX IV contributed to ESS' Massive Open Online Course Accelerate Your Teaching. Targeting high school students, the MAX IV User Office and Communications Group conducted a joint educational project called MAX4MINT, funded by the Swedish Research Council. It attracted over 800 students to MAX IV over 8 months, guided and mentored by MAX IV's student guides. Evaluation surveys showed that the participants increased their knowledge of MAX IV and synchrotron light research and interest in MINT (STEM) topics.

ADMINISTRATION AND SUPPORT

FOREWORD

On the journey towards long-term organisational sustainability, MAX IV's 2023 administrative efforts focused on three main objectives: Filling key management positions, systematically developing administrative processes to enhance efficiency, and gaining a better understanding of economic challenges.

A significant step was the appointment of the MAX IV Director in June 2023, followed by the recruitment of the Head of Communications and the Administrative Director in August. During the autumn, the recruitment process for a new Head of Finance was completed, and she will begin her work in April 2024.

Throughout 2023, administrative working processes were systematically analysed, developed, and refined. The work gave a better understanding of the organisational challenges highlighted in reviews by the Swedish Research Council (VR) and the Internal Audit of Lund University. One improvement was in financial analysis and reporting, which now provides a more reliable basis for decision-making by the MAX IV Board and Senior Management Team. As MAX IV is still transitioning from the development phase to the operational phase, operations costs may be uncertain and must be carefully controlled. In 2023, a thorough analysis of expenses led to a significant reduction in these costs.

Another improvement was in the Organisational and Social Work Environment process, which involved workshops on core values that will result in a Core Value Policy.

The main challenge for MAX IV is to establish a long-term sustainable economic situation. The Senior Management Team implemented various strategies to tackle this issue, including a continued hiring freeze and a process where desirable investments suggested by group managers are prioritised based on MAX IV's Strategic Plan and budget framework.

MAX IV is now progressing towards creating a stable and sustainable organisation with controlled working processes, although there is still work to be done to achieve long-term sustainability.

ORGANISATION AND STAFFING

By the end of 2023, MAX IV employed 293.5 full-time equivalents (FTE) with a total headcount of 313, excluding individuals on long-term leave. The gender ratio was 1/3 women and 2/3 men. Due to the hiring freeze, all recruitment requests were reviewed by the MAX IV Senior Management Team and Board. Any new recruitments or replacements for key positions, including those already granted, were also confirmed by the Senior Management Team before proceeding.

Positions exempted from the hiring freeze in 2023 included Operational postdocs, Floor Coordinators, vacancies in the Accelerator Operations team, and personnel for externally funded projects. All MAX IV vacancies are advertised to targeted national and international networks to attract the most qualified and competent talent. This approach has resulted in the diversity characterising MAX IV's workplace.

Recruitment for key positions

The year began with the recruitment of a permanent MAX IV Director, concluding the interim term initiated in March 2022. Additionally, the position of Administrative Director, also on interim basis, was advertised in early spring. Both positions were successfully filled, with the appointed Director in place by July 1st and the new Administrative Director by August 28th. Other interim positions filled were Head of Communications (employed from August 14th) and Head of Finance (starting April 1st, 2024). By December 2023, the position of group manager in Spectroscopy I remained unfilled.

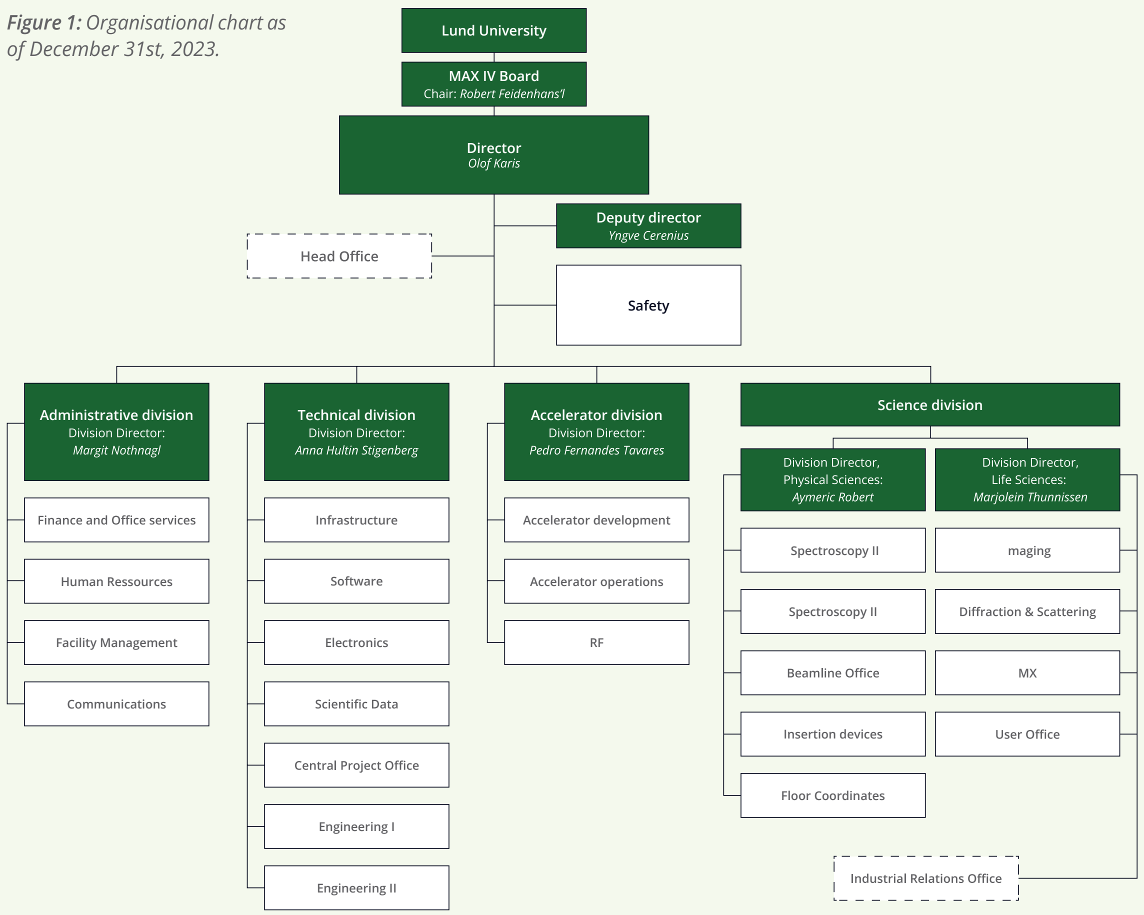
Organisational changes and restructuring

The Technical Division underwent several organisational changes in 2023. The five KITS groups were transformed into four ICT groups: IT Infrastructure, Electronics, Scientific Data, and Software. Four group managers were appointed following an internal recruitment process. The Engineering II group was reviewed, and it was discovered that some tasks it carried out were better suited to other teams. As a result, the Logistics and Technical Services team was removed from the Engineering II group. Three employees joined the Facility Management group, and two joined the Mechanical Workshop team in the Engineering I group.

Two new assistant group managers were appointed within the Safety group for the Experimental Safety team and the Radiation Safety team through an internal recruitment process. They began their assignments on March 1st and April 1st, 2023, respectively. Some of the staffing needs of certain groups were fulfilled by utilising internal resources and optimising the organisational workflow.

The Science Division's planned reorganisation and restructuring, which was decided upon in 2022, will be revisited in 2024 based on continuous discussions and input from the MAX IV Board in 2023.

Figure 1: *Organisational chart as of December 31st, 2023.*



MAX IV's second office space, "The Cube".
Credit: *Wihlborgs/Alexander Olivera.*

Continued move to a second office space

In March 2023, four more groups, including the Industrial Relations Office, User Office, Communications, and Human Resources, moved into MAX IV's second office space, the Cube. Before the move, risk assessments were conducted, and in November 2023, all MAX IV employees were surveyed about their experience of the move. The feedback will be used in conjunction with an inventory of workplace needs and continuous risk assessments to monitor the move's impact.

Core values work and a new onboarding platform

MAX IV is committed to maintaining and enhancing a positive work environment. In the spring of 2023, a bi-annual work environment survey was conducted. Additionally, HR held workshops with all employees to discuss core values. The work resulted in a Core Value Policy to be implemented in 2024. The core values will be integrated into all MAX IV processes, such as recruitment, onboarding, and staff appraisals.

A digital training program has been developed to provide new employees with a better onboarding experience. The aim is to make new employees feel welcomed and included and inform them of their rights and responsibilities in the Swedish government sector. Work will continue with the program and onboarding process in 2024, with the next step being to improve the introduction for managers.

Current financial status and strategic changes

MAX IV is now fully operational, with all phase 1, phase 2, ForMAX, and MicroMAX beamlines being up and running and taking users. The financial situation for the facility is however challenging, with high costs due to several external factors such as increased interest costs and a high inflation rate. This led to increased costs for premises, electricity, and staff.

A special grant from the government as well as financial guarantees from Lund University were both necessary for the decision to continue operations during 2024. The main challenge for MAX IV is now a long-term sustainable financial situation to ensure the facility can continue operating and allow for future growth. As a step in this process, several important strategic measures have been implemented:

- The hiring freeze implemented in 2022 continues, and new positions can only be approved after a formal decision by the Board, which has delegated it to the Head of the Board.
- The budget for travel and conferences has both been reduced and centralised, with a total budget of 5 MSEK to be determined by the Directors.
- A new process for investment and opportunity studies has been implemented, with group managers requesting funding for projects for 2024. The MAX IV Senior Management Team has then prioritised the projects.
- A thorough analysis of the Operations costs with subsequent adjustments and effectivisations has led to a significant reduction in expenses.
- Structural improvements have been made to financial reporting sent to the MAX IV Board as well as more frequent financial follow-ups.

2023 FINANCIAL OUTCOME: TOTAL

Operating revenue (ksek)	Actual 2023	Budget 2023	Forecast 2023	Budget 2024
Government appropriations	85 667	77 375	84 710	91 250
Grants	731 943	718 531	729 682	756 931
Fees and other charges	15 119	7 000	11 616	9 000
Financial	927	200	705	0
Total operating revenue	833 656	803 106	826 713	857 181

Cost (ksek)	Actual 2023	Budget 2023	Forecast 2023	Budget 2024
Staff	-269 956	-273 110	-262 219	-295 598
Premises	-199 884	-212 825	-199 065	-222 900
Operating costs	-83 373	-100 311	-101 843	-81 838
Depreciations	-258 622	-262 878	-255 902	-265 273
LU overhead	-30 681	-30 681	-30 681	-34 989
Financial	-340	-200	-327	0
Total costs	-842 856	-880 006	-850 037	-900 597

Result	-9 200	-76 900	-23 323	-43 416

Table 1: Total financial outcome.

2023 FINANCIAL OUTCOME: OPERATIONS

Operating revenue (ksek)	Actual 2023	Budget 2023	Forecast 2023	Budget 2024
Government appropriations	59 247	63 575	62 527	60 879
Grants	491 021	472 059	496 223	526 219
Fees and other charges	14 566	7 000	10 579	9 000
Financial	767	0	619	0
Total operating revenue	565 601	542 634	569 948	596 098

Cost (ksek)	Actual 2023	Budget 2023	Forecast 2023	Budget 2024
Staff	-246 174	-255 961	-241 953	-272 247
Premises	-189 656	-204 636	-190 259	-210 929
Operating costs	-78 174	-93 411	-97 380	-77 361
Depreciations	-36 130	-38 581	-36 780	-48 963
LU overhead	-26 067	-26 945	-26 664	-30 013
Financial	-261	0	-235	0
Total costs	-576 462	-619 534	-593 272	-639 514

Result	-10 862	-76 900	-23 324	-43 416

Table 2: Financial outcome of operations.

At the end of 2023, MAX IV had a deficit of 9.2 MSEK. This deficit is lower than previously expected due to various cost reductions as well as an increase in grants and efforts to increase revenue through external funding. The number of applications for externally financed projects has increased by 92% compared to last year, as well as an increased revenue of 2 MSEK for proprietary beamtime compared to the budget. In contrast, Swedish universities contributed with 3.8 MSEK less than budgeted, and as more universities now wish to contribute In-Kind this could result in further complications in the future.

MAX IV currently has 802 MSEK in unused funding. There has been a steady decrease in these funds in the last years, mostly due to annual deprecation costs of finished projects. The entirety of these unused funds is tied up in in investments made in the construction of the facility and the beamlines, as well as various projects. Due to the deficit MAX IV also used up almost 10 MSEK of the saved agency capital.

Although the actual costs in 2023 were lower than the budget, there was an actual increase in costs of 109 MSEK compared to 2022. The majority of this is caused by an increase in rental costs of 56 MSEK due to MAX IV's interest-based lease agreement (STIBOR 3M) and an increased electricity cost of 17.6 MSEK. These are significant factors beyond control.

Although the number of employees is approximately the same as last year (294.7 full-time equivalents compared to 300 in 2022), another large factor is an increased cost of 21.8 MSEK for staff. Of these, 11.8 MSEK is due to salary increases, and the remaining 10 MSEK is due to staff moving from construction projects to operations. Both the costs for premises and staff were however lower than the 2023 budget.

Financial outlook 2024 and onwards

MAX IV is currently expecting a small increase in revenue during 2024 compared to 2023. Increased funding from VR (10 MSEK), Treesearch (3.2 MSEK) and Formas (2 MSEK) contributed to this, but the largest boon was the special government grant of 40 MSEK that helped counteract the predicted cost increase for the year. Due to this grant being a one lump sum payment, the forecast of the upcoming years is a continued increase in costs for the facility, but with no expected increase in revenue to balance the finances.

The increase in costs of 2023 is assumed to continue for 2024-2026. Costs such as rent (based on STIBOR 3M) and electricity will continue being high for the upcoming years, these being high risk costs beyond MAX IV's control. The increased cost in staff will continue to affect MAX IV, due to increased salaries and the need to fill critical positions for the continued operation of the facility.

MAX IV has 22.8 MSEK remaining in saved agency capital, but due to the expected deficits this will most likely be used up in 2024. It is therefore critical to increase revenue in order to continue operations.

The recent modification of the ordinance that governs funding granted to research infrastructure of national interest is highly welcomed by MAX IV. The change in the governing documents will allow the Swedish Research Council to grant funding for up to 10 years for MAX IV and similar research infrastructure and aims to reduce financial unpredictability and uncertainty due to short-term funding, enabling more long-term planning and stability. It has the potential to positively affect MAX IV's co-funding stakeholders, partners, universities, and international collaborators, with the opportunity to drive long-term collaborations and investments which will benefit the national research community and society.

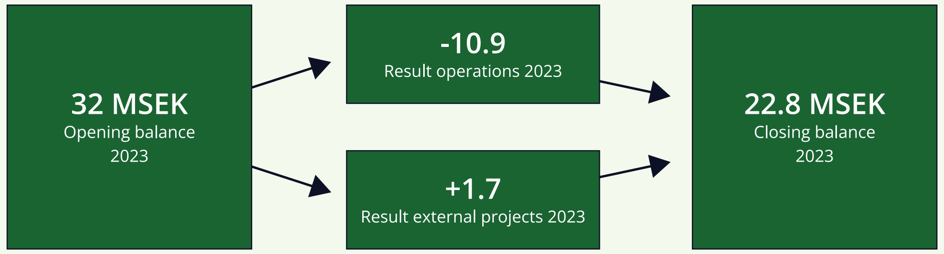


Figure 1: Agency capital 2023.

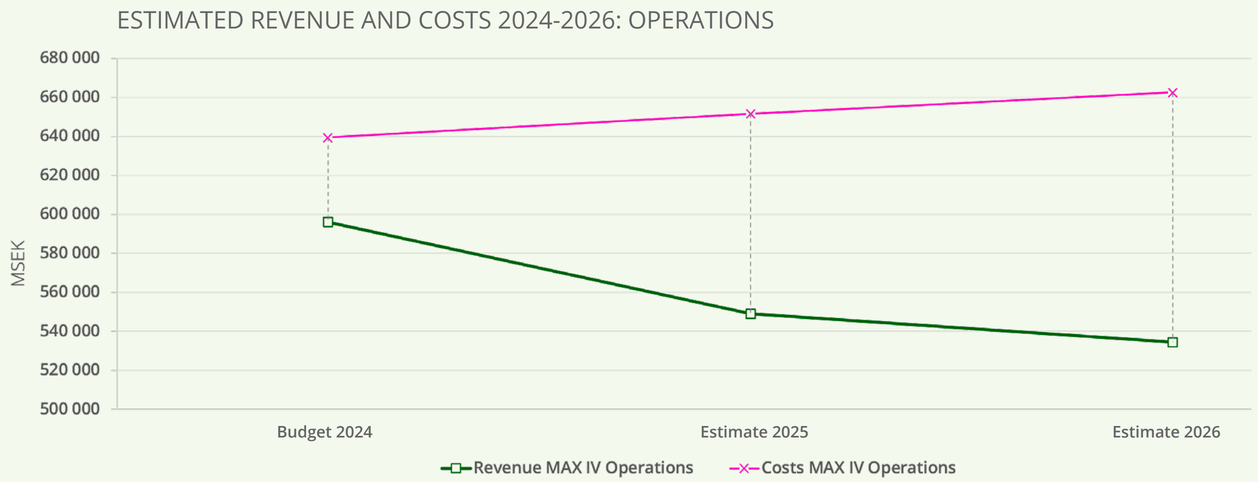


Figure 2: Estimated revenue and costs of MAX IV operations 2023.

LIST OF ABBREVIATIONS

APXPS Ambient Pressure X-ray Photoemission Spectroscopy
ARIE Analytical Research Infrastructures in Europe
ARPES Angle-Resolved Photoelectron Spectroscopy
BAG Block Allocation group
BO Beamline Office
BPAG Beamline Project Advisory Group
BREEAM Building Research Establishment Environmental Assessment Method
CMMS Computerised Maintenance Management System
CCN Cloud Condensation Nuclei
CMOS Complementary Metal Oxide Semiconductor
CPO Central Project Office
CXI Coherent X-ray Imaging
DAQ Data Acquisition
DUV Deep Ultraviolet
ESS European Spallation Source
EU European Union
EUV Extreme Ultraviolet
EXAFS Extended X-ray Absorption Fine Structure
FOFB Fast Orbit Feedback
FTE Full-Time Equivalents
FZP Fresnel Zone Plates
GeV Giga electron Volts
GPU Graphics Processing Unit
GUI Graphical User Interface
HERDi High-resolution powder Diffraction set-up
HR Human Resources
ICT Information and Communications Technology
IRO Industrial Relations Office
KAW Knut and Alice Wallenberg Foundation
KITS Kontroll Information Teknologi System, now replaced by ICT
KTH KTH Royal Institute of Technology, Stockholm
LDM Low-Density Matter
LEAPS League of European Accelerator-based Photon Sources
LED Light Emitting Diode
LU Lund University
M1 First Mirror
mA Milli-Ampere
MIK Multipole Injection Kicker
MSCA Marie Sklodowska-Curie Actions
MSEK Million Swedish Kronor
MTBF Mean Time Between Failures
MX Macromolecular Crystallography
OER Oxygen Evolution Reaction
PLC Programmable Logic Controller
PAC Programme Allocation Committee
PGS Plane Grating Spectrometer
Pmrad Picometer-radian
PRISMAS PhD Research and Innovations in Synchrotron Methods and Applications in Sweden
RFI Council for Research Infrastructure
RISE Swedish Research Institutes of Sweden
RIXS Resonant Inelastic X-ray Scattering
SAXS Small Angle X-ray Scattering
SME Small and Medium-sized Enterprises
SMS Surface/Material Science
SOFB Slow Orbit Feedback
SPELEEM Spectroscopic Photoemission and Low Energy Electron Microscope
SPF Short Pulse Facility
STIBOR Stockholm Interbank Offered Rate
STXM Scanning Transmission X-ray Microscopy
SU Stockholm University
SWAXS Small- and Wide-Angle X-ray Scattering
SXL Soft X-ray Laser
TDC Transverse Deflecting Cavity
TREM2 Triggering Receptor Expressed on Myelin Cells 2
TRIBs Transverse Resonant Island Buckets
TRISS Trapped Ion Spectrometer Setup
TRL Technology Readiness Level
Vinnova Swedish Governmental Agency for Innovation Systems
VR Vetenskapsrådet, Swedish Research Council
WAXS Wide Angle X-ray Scattering
XANES X-ray Absorption Near-Edge Structure
XAS X-ray and Absorption Spectroscopy
XES X-ray and Emission Spectroscopy
XFEL European X-ray Free-Electron Laser Facility
WISE Wallenberg Initiative Materials Science for Sustainability
XMCD X-ray Magnetic Circular Dichroism
XPCS X-ray Photon Correlation Spectroscopy
XPS Flexible Photoelectron Spectroscopy
XRD X-ray Diffraction
XRF X-ray Flourescence

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