PETRA III Swedish Node

Center for X-rays in Swedish Materials Science

2021 Organisational Report

Diarienummer 4.3-2018-06942

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April 2022

The project is funded by Swedish Research Council

Preface

Synchrotrons are considered to be a key research tool, which can enhance our understanding of material properties - both in fundamental and applied research.

Sweden has therefore invested significantly in such research infrastructures. Such investments include the MAX IV facility in southern Sweden as well as the PETRA III facility, Hamburg, Germany.

The investments at PETRA III have been undertaken as part of various contracts between DESY and the Swedish Research Council (VR). Firstly, Sweden commissioned the building of a Swedish Material Science Beamline; and, from autumn 2019, there is a contract between DESY and VR that provides Swedish organisations with 5300 hours per year of privileged access to beamlines at PETRA III.

The monitoring of Swedish access rights, and general safeguarding of Swedish interests at PETRA III, has been tasked to the host universities KTH and Linköping University - who have established the Center for X-Rays in Swedish Materials Science (CeXS) for this purpose. CeXS ought to also undertake outreach and educational activities.

The inauguration of CeXS was held in August 2019. The Swedish Material Science beamline was commissioned and become fully operational during 2019.

Together CeXS, the Swedish Material Science Beamline and the virtual beamline with Swedish privileged access comprise the PETRA III Swedish node.

This report provides information about Swedish interests and use of PETRA III as well as key CeXS activities during 2021.

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Summary

Proposal submission data shows sustained Swedish research interest for using PETRA III. During 2021, Swedish universities, research institutes and companies submitted 144 beam time proposal.

Of these proposals, 41 (28.5%) were for use of the Swedish Material Science beamline.

During 2021, 58 beam times projects were completed:

- 46 beam times (80%) had a university project lead
- 6 beam times (19%) had RISE/Swerim as a project lead
- 6 beam times (8.5%) had a company as project lead/were undertaken on a commercial basis

Of the 52 open access beam times, 38 were granted on the basis of Swedish privileged access, and another 14 were granted beam time since they were still more competitively ranked than other international proposals.

Despite the COVID-19 restrictions, during 2021, 173 Swedish users visited PETRA III to undertake measurements, 58 Swedish users accessed data at PETRA III and 17 users participated in remote measurements.

38 publications were reported to the DOOR system by Swedish users during 2021. This is likely to reflect the limited number of beam time projects conducted in 2020 due to the effects of pandemic restrictions.

Concerning development of the Swedish beamline's experimental capabilities, there is continued engagement by CeXS and the beamline managers on developing experimental environments.

DESY's project to upgrade PETRA III to its fourth generation is proceeding. The situation is still fluid, with CeXS continuing the dialogue with the upgrade project and arranging briefings for the Swedish community.

CeXS organised and held community briefings, events and educational initiatives as well as contributed to educational activities organised by industry and research institutes.

Proactive dissemination of PETRA III Swedish Node information via direct mails, briefings, the upgraded CeXS homepages and the CeXS LinkedIn site occurred throughout 2021.

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1. Background

Sweden has invested in the construction of a Swedish Material Science beamline (SMS), with two branches (P21.1 and P21.2), at the PETRA III synchrotron in Hamburg, Germany. This became operational during 2019.

From 2019, researchers affiliated to Swedish organisations have also had 5300 hours of privileged access to all DESY operated beamlines at PETRA III.

In connection with these investments, the Center for X-Rays in Swedish Material Science (CeXS) was established to act as the academic host of the Swedish Material Science beamline.

Furthermore, the Swedish Research Council (VR) has tasked CeXS with securing Swedish interests at PETRA III and collecting data about a) Swedish use of PETRA III and b) international's use of the P21 beamline at PETRA III.

CeXS should also arrange workshops and disseminate information about PETRA III opportunities to the Swedish material science community.

Together CeXS, the SMS beamline and virtual beamlines via privileged access constitute the PETRA III Swedish Node.

For 2021, a year characterised by the ongoing COVID-19 pandemic, this report provides information relating to these tasks.

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2. The PETRA III Swedish Node's organisational entities

CeXS was inaugurated in August 2019 and established an organisational structure from 2020, which functioned throughout 2021.

2.1 The PETRA III Swedish Node's organisational entities

CeXS Management Team

CeXS activities continue to be planned and implemented by the following people:

- Director. Peter Hedström. KTH. 0.3 FTE
- Vice Director. Fredrik Eriksson. LiU. 0.3 FTE
- Manager. Denise McCluskey. KTH. 0.5 FTE

A post doc (0.5 FTE) has been carrying out supporting development duties from June 2021.

CeXS Board

The management team reports to a board, which sets the direction for CeXS. Board members are:

- Jens Birch (LiU), Chair
- Mikael Östling (KTH), vice Chair
- Per Dannetun (LiU)
- Annika Borgenstam (KTH)
- Ulrich Lienert (DESY)
- Conny Såthe (MaxIV)

The board met on 21 January, 8 September and 28 October 2021.

Figure 1 illustrates the above CeXS organisation as well as the governance stipulated by the VR-DESY contract.

Representation on governance fora

The VR-DESY contract stipulates two governance fora.

- The Steering Committee, which has one CeXS nominated representative, who is Prof. Ulf Karlsson (2020-2021).
- The Steering Group comprises only CeXS nominated representatives. As reported for 2020, two of these representatives are the director and vice director of CeXS and the third is Assoc Prof Lina Rogström (LiU).

The Beamline Steering Group meeting was held on 26 March.

CeXS reminded DESY also during 2021 about the need to organise and hold regular meetings of the Beamline Steering Committee.

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2.2 DESY's organisation and processes

The P21.1 beamline branch is managed by Dr. Martin von Zimmermann and run by him and a staff of 2 FTE beamline scientists. The P21.2 beamline branch is managed by Dr. Ulrich Lienert and run by him and a staff of 4 beamline scientists. For their respective beamline branches, Drs. Lienert and von Zimmermann have overall responsibility for planning beamline use, supporting users at the beamline as well as planning beamline maintenance and instrument upgrades.

Beam time allocation, including privileged beam time access, is decided as part of DESY's call process. The person responsible for that process is DESY's Dr Oliver Seek. DESY makes a call and researchers submit proposals for beam time access. Proposals are assessed on the basis of scientific excellence and project feasibility by independent scientists. Scientists then meet together in a so called Project Review Panel (PRP), which ranks proposals, with the ranking being the basis for beam time prioritisation. (see this CeXS homepage for a fuller description of that process).

There are various PRPs for differing beamlines (see this DESY site for more information about the PRP beamline groupings and members). CeXS has taken an active role in identifying and providing lists of suggested candidates for the PRPs to DESY, which DESY then select from. Currently there are 9 Swedish representatives on 8 of 13 PRPs.

Note. In order to be proactive in safeguarding Swedish interests, CeXS requested that we observe the PRP that involves the SMS beamline. This occured in 2020. DESY however became concerned about confidentiality issues. Therefore, in 2021, the process of pro-actively monitoring and advising on the allocated privileged access process was changed.

2.3 Joint CeXS and DESY Processes

With regards privileged access, the new process is:

- DESY emails CeXS extracts of the beam time proposals that select 'Swedish privileged access' in the DOOR submission portal shortly after the deadline
- CeXS screen the proposals, ensuring the eligibility criteria that the project leader is affiliated to a Swedish organisation is fulfilled
- DESY then hold a meeting with CeXS, where they step through the privileged access allocation. We see that, beamline by beamline, eligible proposals whose ranking fell below the cut-off threshold are

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tentatively allocated beam time access up to the maximum allocation threshold agreed in the VR-DESY Cooperation Agreement. That is, 25% at most beamlines, 50% at the P21.1 branch and 100% at the P21.2 beamline branch.

- Actual beam time allocation is then subsequently anchored with the responsible beamline managers as there may be details that need to be confirmed
- CeXS subsequently receives the list of allocated privileged access beam times.

CeXS intervened in 2-10% of proposals because they do not fulfil the eligibility criteria that the project leader ought to be affiliated to a Swedish organisation. Reasons for non-eligibility are typically:

1. Proposals have German leaders and co applicants. However, the beam time is one part of a larger project, which is funded by RÅC
2. Proposals have Swedish co-applicants. However, the project leader is not affiliated to a Swedish organisation.

Lists of privileged access proposals were received in April and November.

Meetings to step through the privileged access allocation across the beamlines were held on 10 June and 11 November 2021.

2.4 Use of income from paid industry beam time

During 2021, CeXS secured an agreement with DESY that funds from paid industry use of the Swedish beamline would be used to hire a beamline scientists. That scientists would be dedicated to providing industry with additional support.

DESY initiated a hiring process in the autumn. This new position was advertised on DESY's home page, CeXS homepage and CeXS linked-in pages during 2021. CeXS also emailed all Swedish universities informing them of the position and requesting that they forward the job announcement to relevant people in their network.

The new recruit is expected to start in 2022.

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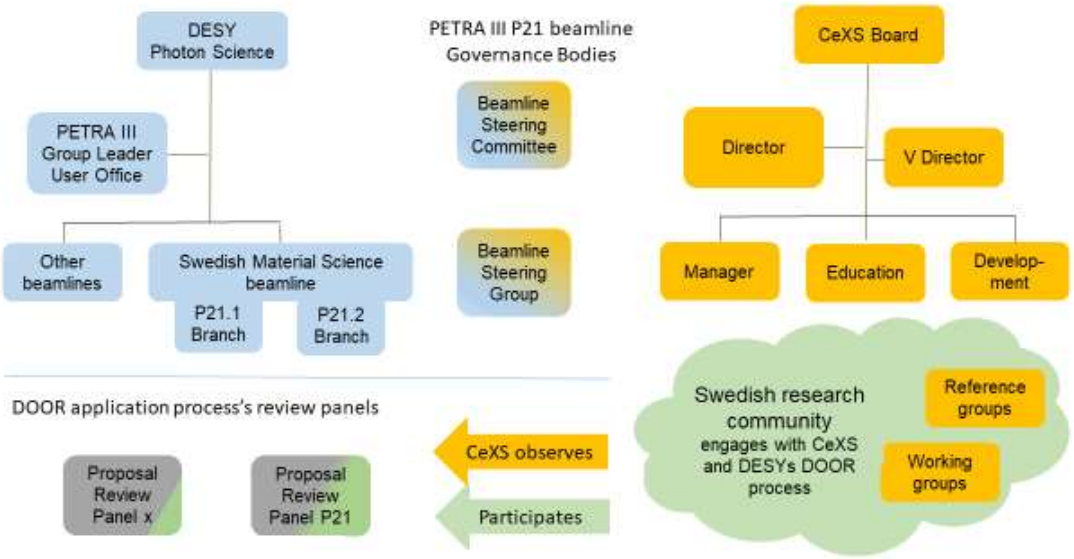

Figure 1. Academic hosting of the Swedish Material Science beamline and governance of the VR-DESY contract.

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3. Data sources concerning Swedish use of PETRA III

1. Extract of proposals that had selected the “applying for privileged Swedish access” in the DOOR system
   This option became available during 2019. Extracts contained the name and organisation of the project leader, principal investigator and co-proposers as well as the proposal’s abstract, requested beamline and the method/experimental setup.

2. Lists of proposals that were granted beam times on the basis of Swedish privileged access

3. List of articles, based on measurement data from PETRA III, with Swedish authors that were published during 2021 – and actually registered in the DOOR system.

4. Statistics about proposals, organisations and gender as well as statistics about granted beam times, and number of users (see the complementary excel spreadsheet. For 2021, the spreadsheet contents were produced by DESY’s IT support organisation extracting information from DOOR. DOOR is the system used by DESY to manage beam time proposal submissions, user information and granted beam times, as well as which users actually access the DESY facilities and how they access those facilities.)

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4. PETRA III: Submissions and approved projects

The DESY beam time calls that enabled open research access to PETRA III during 2021 had deadlines in September 2020, March 2021 and possibly September 2021. However, due to Covid-19 disruptions, the September 2020 call was only open to proposals for 6 of the 18 beamlines[1].

DESY continued to operate the PETRA III facility under the ongoing pandemic. Researchers essentially had to present negative tests. Furthermore, the number of participants at each beam time was often constrained to 3 people.

Proposals and awarded beam times

The September 2020 call received 6 eligible Swedish privileged access proposals, the March 2021 call received 78 eligible proposals and the Sept 2021 call received 56 eligible proposals.

118 proposals had project leaders affiliated to a Swedish university, 11 to a research institute and others were affiliated to a company. Overall 58 beam time were undertaken. That is, 40% of proposals were successful. For comparison, the number of completed beam times during 2020 was 37 due to the impact of the pandemic.)

Of the 144 proposals, 24 (19%) had a female project leader. 18% of the proposals awarded beam time had a female project leader. Of the 673 people listed as project leader, principle investigator or co-proposer in proposal submissions, 148 (22%) are female. Of the proposals awarded, 40 (23%) of the 175 applicants are female. Accordingly, female participation rates in this field are low. However, gender parity is maintained vertically as well as over in the beam time allocation process.

The most requested beamlines was the Swedish beamline, with P21.2 branch attracting 26% of Swedish proposals and the P21.1 branch 4%. Thereafter the P22 beamline attracted 22% of proposals, P03 beamline 11% and P07 beamline 9%. All PETRA beamline received at least one or two proposals at each call. Accordingly, there is a sustained demand for privileged access to all beamlines as well as a sustained high demand for the SMS in this period.

Swedish industry's paid use

Swedish companies paid to undertake 6 beam time projects at PETRA III during 2021. Two of these were at the Swedish beamline.

Types of access

In practice, 173 people that were granted access to PETRA III facilities actually used the facilities on site i.e. for beamline measurements. A further

[1] P01, P09 (for a few setups), P11, P24, P61 (HZG hutch only), P65

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17 people conducted beamline measurements remotely. An additional 58 accessed experimental data. Some of these people may have been on site. Some not (DESY doesn't distinguish). It is a common occurrence that some people don't attend the beamline experiment but get involved in the data analysis.

5. The Swedish Beamline: Submissions and projects

Of the 144 proposals submitted to PETRA III during 2021, 41 proposals (27.7%) requested to use the Swedish Material Science beamline. This compares to 18.5% in 2020. A total of 14 beam times were granted and used.

11 of these were from academia, 2 from companies and 1 from institutes. Of the 41 proposals requesting use of the Swedish beamline, 7 (17%) had a female project leader. Of the 14 proposals awarded beam time, 3 (21%) had a female project leader. Of the 158 people listed as project leader, principle investigator or co-proposer in proposal submissions, 37 (23%) are female. Of the proposals awarded, 13 (24%) of the 55 applicants are female. Accordingly, female participation rates in this field are low. However, gender parity is maintained over in the beam time allocation process.

6. PETRA III Users' publications

The number of peer review publications involving measurement data at PETRA III, where one of the authors was affiliated to a Swedish organisation and the paper was also registered in the DOOR system, was 34 in 2021, 88 in 2020, 60 in 2019 and 53 papers in 2018. The low publication rate in 2021 could be attributed to the limited number of beamtime experiments that were possible during 2020 due to the stringent restrictions enforced during 2020. However, publication rates are likely to be underreported.

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7 CeXS Strategy Area 1. Competences

During 2021, CeXS organised three competence development events for the Swedish Material Science research community.

22 January SMS Satellite Meeting online

On 22 January, CeXS and the P21.2 beamline manager jointly organised and held a SMS satellite meeting at PETRA III. This was attended by 30 researchers from the Swedish community. The agenda was beamline updates, emerging research results from the Swedish community, and a discussion of topics of interest to the community, especially education and training. There was also a visit to the beamline.

19-20 October Hands-on Stress/Strain Data analysis workshop

When the pandemic restrictions eased, CeXS organised a hands-on workshop on stress-strain data analysis. This was held at the Tekniska Museum in Stockholm. On 19 Oct, after an introductory session, researchers presented their stress-strain experiments and data analysis challenges. On day 2, industry researchers, post docs and PhD students carried out two data analysis exercises. 31 people participated. The event was well received, with people reporting that they feel more confident in undertaking data analysis after having performed the exercises. This workshop was co-organised by the MetaLSF project that is sponsored by EIT RawMaterials.

17 November Introduction to PDF and research opportunities

Swedish researchers are not particularly familiar with the PDF method and types of experiments that are possible at the P21.1 beamline branch. The beamline manager and staff therefore kindly agreed to hold an online lecture that introduced the PDF technique. A second lecture gave an overview of some research experiments that had been conducted at the P21.1 branch.

8 CeXS Strategy Area 2. Capacity

19-20 October Hands-on Stress/Strain Data analysis workshop

This event reported above target people new to synchrotrons and so functioned as a capacity, as well as a competence development, activity.

11 November CeXS at Malmö Live

This IRL event was coorganised by CeXS, Lund University and Malmö University. It targeted people who were new to synchrotron research, providing a popular science overview of the experiments and their research outcomes. There were 30 participants.

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9 CeXS Strategy Area 3. Infrastructure

29 June Review of sample environment specifications

DESY has a budget to procure a sample environment - a furnace - for the Swedish material science beamline, P21.2 branch.

The experimental needs of the Swedish materials research community has been assessed, and proposed specifications for a furnace sample environment developed, by a working group comprising Dr Ulrich Lienert (DESY), Docent Magnus Colliander (Chalmers) and Professor Peter Hedström (KTH and CeXS).

CeXS and the working group were inviting the Swedish research community to review the proposed specifications as well as provide additional input.

There were 30 participants.

1 September Briefing concerning PIV and the Sweden Inventory

This briefing addressed the Swedish Research Council's bi-annual infrastructure inventory update (6 Oct deadline) concerning the Swedish material science community's beamline infrastructure needs at the future PETRA IV. The status of the PETRA IV project was presented by Prof Christian Schroer, DESY. Scenarios for implementing the Swedish SiPs were also discussed. This enabled the Swedish community to give input to the proposals submitted by CeXS.

There were 25 participants.

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10 CeXS Strategy Area 4. Gender

CeXS and PETRA III operations are primarily undertaken by professionals with level 2 and above degrees. At this level, in the Science and Engineering sector, there is a recognised gender imbalance with female representation being at most 20-30% and declining to 20% at professor level. Female representation rates in the use of PETRA III at similar levels. The percentage of female project leaders who are awarded beam times is at the same level as the percentage of proposals with female project leaders.

CeXS Board

CeXS board membership at professor level. One in six (16.7%) of the Board are female. This representation reflects the level of gender inequality in Science & Engineering disciplines within the Swedish University sector.

CeXS will take action during 2022 to increase female representation on the Board.

CeXS Management team

One in three (33.3%) of the CeXS Management team is female. This representation reflects the level of gender inequality in Science & Engineering disciplines within the Swedish University sector.

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11 CeXS Stategy Area 7. Communications

An article about CeXS was published in Bergsmannen in February.

Participated in the IVA/RISE Make Use event on research infrastructure as a rapporteur and as experts.

Briefed Tobias Krantz regarding the government enquiry into long term funding of national research infrastructures.

CeXS now has a professionally designed logo.

CeXS homepages have been redesigned, including the new logo. The range of content has been extended. News/calendar is continually updated.

CeXS linked-in continues to post regularly.

CeXS entry in the Swedish Guide has been updated.

CeXS engaged with MAX IV and ESS in a dialogue about the MAXESS Industry Arena portal. Our intent with the dialogue is to raise awareness of the need to demonstrate the complementarity of MAX IV, ESS and the PETRA III Swedish Node.

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12 Budget

CeXS ramped up its activities in 2021 and will continue to ramp up during 2022. Our current under spend will therefore be resolved.

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