REPORT ON THE PROGRESS AND DIRECTION OF RESEARCH AT MAX IV

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As requested by Vice Chancellor, Prof. Torbjörn von Schantz, Lund University, the enclosed document gives a short report on the progress and direction of research at MAX IV, based on the information available to MAC and SAC.

Executive summary

The MAX project is presently developing from a national laboratory with very significant impact worldwide based on a small dedicated staff with modest resources into a large-scale international laboratory with high ambitions using a fairly large, recently hired staff and relatively large resources. MAC and SAC emphasize that very significant progress has been made at MAX IV recently. The following points summarize the current progress of the MAX IV laboratory:

1. The accelerator and storage rings of MAX IV are operating well. 24/7 operation of the accelerators is in place, which is a prerequisite for success.
2. Scientific results are appearing and beamlines are entering operational phase. Three beamlines are currently in user operation.
3. The framework for user support for beamlines in user operation now needs to be established and settled.
4. Most beamlines are delayed compared to original plans. Whether the available resources and the ambitions of the lab are matched is not fully clear, but the delays already encountered for the first beamlines raise concerns.
5. Choosing and keeping priorities, while keeping all staff onboard and maintaining the feeling of being an indispensable part of the big facility is challenging during the transition from the construction to the operational phase. It is particularly important in the current situation, with a very large number of beamlines being in various phases of development.
6. The overall resource situation at the laboratory needs consideration given the ambitious plans of the facility. A resources loaded schedule, and follow-up, for the facility operation and development is an essential tool for defining future priorities. A review of such a schedule by an external committee may also be worth considering.

1. The MAX IV MAC and SAC modes of operation

The Terms of reference of MAC and SAC are enclosed in Appendix 1, including the current members of the two committees.

MAC meets at MAX IV once a year, in May-June. The agenda, decided by the chair together with the MAX IV management, typically includes the status of commissioning and operation of the MAX IV accelerator complex, as well as its strategic development and mid- to long-term upgrades. A report is written based on these meetings. The last two reports are enclosed, Appendix 2.

The current SAC was appointed by the MAX IV Board in spring 2017 and has two meetings per year, in May-June and October-November. The meetings are usually 2 half-days. The points on the agenda are decided by the SAC chair and the MAX IV management and include a status report, beamline updates as well as questions and issues requested by SAC during the previous meeting. The SAC agenda always includes direct feedback from beamline staff, as was decided during the first meeting of the current committee in May 2017. A written report is submitted to the MAX IV management based on the discussion during the meeting, which includes a number of specific recommendations to the facility. The reports from the three meetings of current SAC are enclosed, Appendix 3. Also enclosed, Appendix 4, is the written response from the MAX IV management on the SAC June 2018 report.

2. Progress and research direction of the accelerator system

The pioneering work of the MAXIV team has delivered the first storage ring light source approaching the diffraction limit for keV photons, enabling the commissioning and initial experiments on the first beamlines. The accelerator complex is in almost full operation, delivering light on a 24/7 basis. Still pending is 10 Hz operation of the linac for FemtoMAX, with a further increase to 100 Hz planned in the future. The most important machine conditions to make this source a success have been demonstrated: operation with top-up injection and very high reliability, extremely good base stability, high currents in both rings, and very short bunches in FemtoMAX. Of course many details of the accelerator systems and their beams are still to be investigated and worked on over the coming years. These concern both the details of the beam stability and operation, but further adjustments will also be needed as additional insertion devices and their beamlines are taken into operation. It will here be important to minimize the cross-talk from gap changes in one insertion device to other beamlines.

Moreover, the accelerator staff together with the operations staff seem to us to be suitable for this mode of operation and minor future improvements. Although MAX IV has taken the lead in developing the brightest light source in the world, others are already planning even better sources. Clearly, there is a wish for MAX IV to stay in the lead, and the present design certainly contains some unexplored potential. Furthermore, a design study for a new free-electron laser at the laboratory exploiting the 3-GeV linac is currently underway. The MAC encourages such developments as long as it does not compromise beam delivery to the many experiments which have to be given priority at this stage. At present, the overall goal must be to exploit the huge potential and huge investment in the new laboratory by producing excellent science and technology for the benefit of Sweden and the world.

3. Progress and research direction of the different MAX IV beamlines

MAX IV as an international and national facility serves dual purposes, excellence and more general access to synchrotron radiation for Swedish users, respectively. This is reflected in the beamline and endstation portfolio of the facility and means that the laboratory both accommodates cutting edge science as well as high quality science performed by a broader research community. Doing both – developing highly specialized instrumentation while covering a very wide range of science – is challenging for any facility. Most facilities focus on a few selected areas of excellence. MAX IV is more ambitious by providing three accelerators (1.5 GeV ring, 3 GeV ring and linear accelerator) and suite of beamlines covering and providing access for a broad research community. This is a very tall order and it requires careful consideration with respect to development of the facility and its available resources. Moreover, at some beamlines a large number of sample environments are planned reflecting the goal to accommodate all users, illustrated by the case of HIPPIE below.

3.1 Status and progress of the MAX IV beamlines

At present 16 beamlines have been funded. The status, divided into "user operation", "commissioning" and "construction", of the different beamlines is illustrated in Figure 1, as well as their location at the two storage rings and the linear accelerator. Currently, three beamlines are in user operation, five in commissioning and eight under construction. Two beamlines planned in the next phase, DIFFMAX and MEDMAX, are not yet funded. The different beamlines and their status and progress are presented below. Some more detail on the different timelines are given in the enclosed document submitted by the MAX IV management to the Swedish Research Council (VR) in May 2018, Appendix 5. SAC was given this information during the meeting in June 2018.

An issue which has been high on the agenda of SAC is the 24/7 operation of the MAX IV facility. This is imperative to the success of the laboratory and is, as stated above, now in place. At the meeting June 7-8 2018 SAC learned that agreements with the labour unions with respect to user support at beamlines during user operations are still not settled. Resolving this issue is essential for the operation of the beamlines now in user operation as well as for the beamlines soon to enter this stage. SAC strongly recommends that MAX IV adopts a user support scheme similar to that in operation at other synchrotron facilities. Such a state-of-the-art facilitiy should be able to offer at least on-call user support 7 days a week from morning (8am) to about 10pm during experiments. Developing an agreement with the labour unions on this issue as soon as possible will be crucial for the success and reputation of MAX IV. The response from the MAX IV management on this SAC recommendation is: "This is a good ambition, but MAX IV has limited operational resources. Some things that are standard at other facilities are not possible for MAX IV. A careful analysis of the operations budget will be required to evaluate how to best use the resources according to the mission and how much of this recommendation can be implemented". For reference, 4 persons per beamline is the usual number at SOLEIL, ALBA and ESRF.

3.1.1. Beamlines in user operation

As of June 2018, three beamlines at MAX IV are in user operation, BioMAX, HIPPIE and NanoMAX. Though these three beamlines are in user operation, they are still not fully developed, but are now in a ramp up phase (denoted phase 3 in the document in Appendix 5), during which some commissioning is still ongoing. The timeline and resource allocation for

these developments need to be clearly included in the plans laid out by MAX IV. The status of these three beamlines is shortly presented in the following.

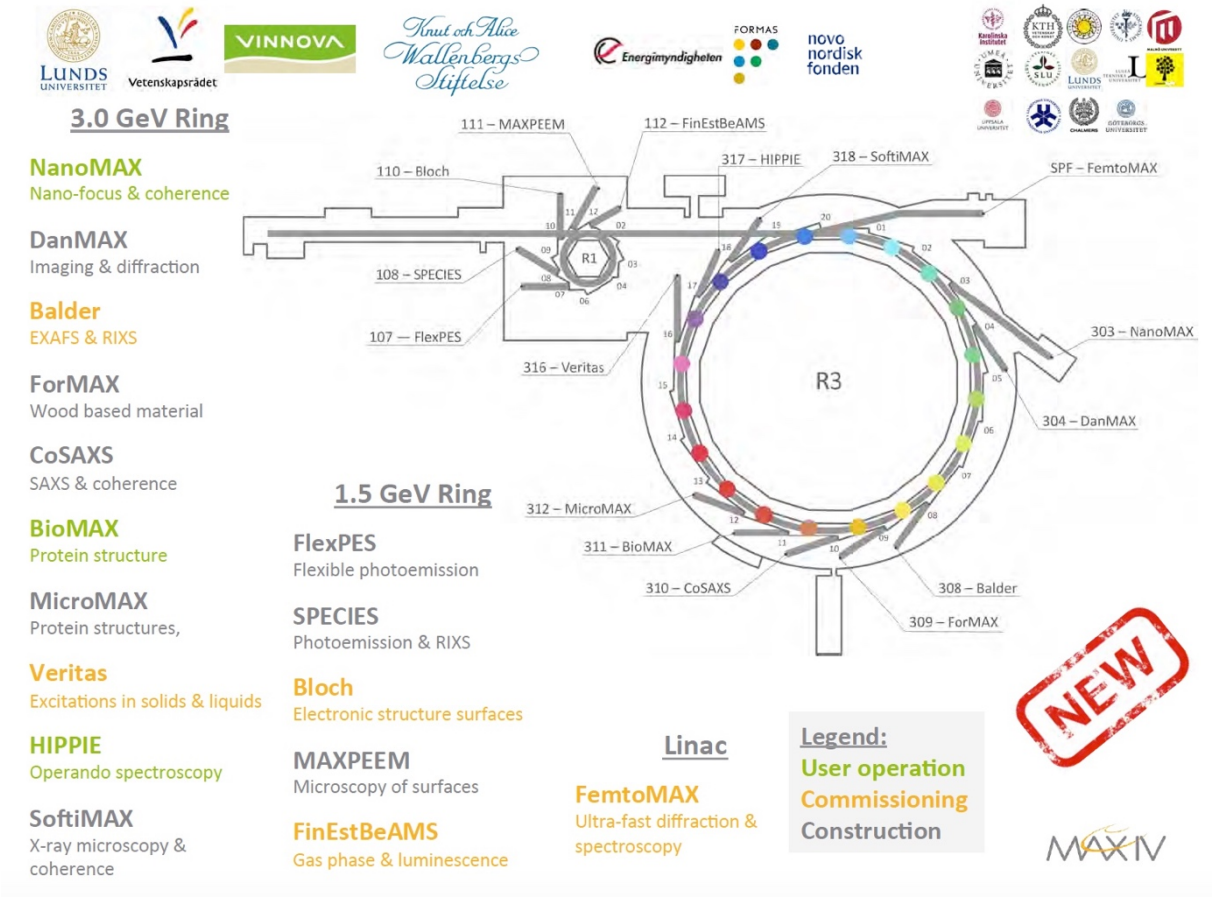

Figure 1. Schematic view of the currently funded beamlines at MAX IV. The figure is taken from the presentation by Director Christoph Quitman during the MAC/SAC meeting June 7-8 2018.

BioMAX

BioMAX took on 6 expert user groups and 6 regular user groups before summer 2017. This was according to the schedule for opening of this beamline to users. The beamline is currently in regular user operation and has also introduced Block Allocation Group (BAG) proposals, standard in the macromolecular crystallography (MX) community, which is important for the competitiveness of this beamline and to enable MX user groups to make the best use of awarded beamtime. SAC finds that the beamline team has a clear vision and is making excellent progress. Development of the beamline is running in parallel with the user operation. The quality of the beamline is also recognized by industrial users. Serial crystallography experiments have quite recently been implemented. The move towards remote operation that is currently being pursued is also very important for the progress of this beamline. The beamline is already productive, with a first user publication and structure

deposited in the PDB (Protein Data Bank). It should be noted that structural biology papers usually also require considerable non-structural data and this often results in a delay in publication, even after a successful beamtime. This is a common challenge for all MX beamlines. BioMAX is already attracting both industrial (3 companies) and academic (38 groups) users with strong scientific proposals. This puts them well on track for this stage of their development in comparison to peer facilities and will lead to an increasing number of high-impact papers as user projects mature. SAC is particularly pleased to see that the beamline team are embracing recent developments in sample delivery and environment (i.e. serial and room temperature data collection) as these are increasingly in demand from users at all facilities. Commissioning work still remains to be done, particularly on the robotic sample changer as well as the serial crystallography sample environments and it will be important to ensure the team have time and resources for this. Absolutely vital is that BioMAX is able to offer remote operation as soon as possible.

HIPPIE
HIPPIE was opened for users at the end of 2017. Originally, the beamline was planned for user operation from March 2017. Some delays due to limited controls and IT (KITS) resources were reported to SAC in November 2017. The beamline is currently in regular user operation. SAC finds that the beamline is making excellent progress. HIPPIE is a state-of-the-art near ambient pressure photoelectron spectroscopy beamline. The beamline can accommodate a range of sample cells. So far, the catalysis cell and the electrochemical cell have been implemented. Thus, primarily catalysis experiments have been performed at this point. Publications are about to appear from this beamline. HIPPIE is a beamline with high scientific potential, and SAC expects this to be evident in the near future in the form of high-impact publications.

The beamline has the potential to reach a broader user community, for example by installing a fast loading cell for biological and geological applications. However, such new cells require more manpower than is currently available as well as long turnover times, putting limitations on the beamtime scheduling. SAC has therefore at this point recommended that the beamline concentrates their efforts on a limited number of sample cells to make sure that these are operating according to user expectations.

The plans for different sample cells at HIPPIE illustrate the dilemmas/challenges facing MAX IV with respect to the wide scientific scope of the facility. A total of 7 sample cells/environments are planned for the beamline as a response to requests from a broad user community. The MAX IV management should very carefully evaluate, in collaboration with the SAC, how many different sample environments make sense and are reasonable for each beamline, i.e. are the resources available to build and then operate all these capabilities.

The syngery between HIPPIE and SPECIES, who have similar scientific cases, could be exploited more and – in the long term – MAX IV management should divide specific scientific areas (and sample cells) between the two beamlines.

NanoMAX
NanoMAX is a beamline which fully utilises the coherence and brightness of the MAX IV facility and thus is a showcase for the capabilities of the facility. It has been open for users at one of its two experimental stations since May 2017. Giving priority to one of the two experimental stations, the Kirkpatrick-Baez (KB) optics station, was strongly advised by SAC to ensure user access as early as possible. This recommendation has been implemented. Two

papers describing technical aspects of the beamline are published, however, to the knowledge of SAC, scientific results from user experiments are yet to appear in literature. SAC emphasizes that this beamline has strong scientific potential. Research topics that can be accommodated at NanoMAX are diverse, including timely questions in materials science, life science, earth science, nanoscience, physics, chemistry and biology. The MAX IV facility provides X-ray beams with up to 40 times larger coherent fraction, depending on the photon energy, than other synchrotron sources currently operating around the world. This means that X-ray microscopy will be very efficient at NanoMAX once the beamline is working at its full potential, enabling very high spatial resolution at much higher speed compared to what is possible to do today. SAC has recommended that NanoMAX focuses on a demonstration experiment that shows this unique capability, which in turn should initiate high impact research. SAC has also recommended a plan be made for the further development of this beamline.

3.1.2 Beamlines in commissioning phase

There are a number of beamlines in the commissioning phase at present; Balder, BLOCH, FemtoMAX, FinEstBeAMS and VERITAS. Among these BLOCH, FinEstBeAMS and VERITAS, all located on the 1.5GeV ring, have obtained their radiation safety permit. A call for commissioning expert users has been opened for BLOCH and FinEstBeAMS.

BLOCH and FinEstBeAMS will serve the traditionally strong soft X-ray spectroscopy community that existed at MAX-lab. BLOCH has two branches covering high resolution angle-resolved photoelectron spectroscopy (ARPES), with optionally spin resolved (Spin-ARPES) and core level spectroscopy, experimental techniques serving excellent Swedish research groups with long traditions in developing these methods. FinEstBeAMS also has two branches and three endstations covering gas phase spectroscopy, fluorescence spectroscopy and solid state spectroscopy. The latter endstation is under construction while the two others are part of the current commissioning. The beamline serves in particular strong Nordic and Baltic user groups. Both beamlines are delayed by approximately one year compared to the original plans, but SAC expects these two beamlines to make good progress during the coming year.

FemtoMAX has been operating at 2 Hz but is designed for 100 Hz operation. Currently, 10 Hz is the target, which opens good scientific opportunities but requires a radiation safety permit to be in place. This beamline is built for investigating ultrafast phenomena in physical and life sciences and holds a unique niche in the scientific landscape. The beamline team has worked on all issues that they can control, including achieving a scientific publication based on results from the beamline. Currently access to KITS resources in addition to the radiation permit for 10 Hz operation is limiting further progress. FemtoMAX is not among the beamlines highest on the priority list, as motivated in the response to the SAC recommendations in Appendix 4, and the MAX IV management estimates a delay of about 2.5 years compared to the original plans.

The Balder beamline has been severely delayed for a number of reasons, which has been an ongoing concern for SAC. In its November 2017 meeting SAC recommended that “the beamline team move ahead with the parts that can be built (i.e. spectrometers, realistic testing of analyzer crystals, experimental chambers and environments) while they are waiting for the beam path installation and define a minimal configuration that is required to enter user operation”. SAC learned during the meeting in June 2018 that the BALDER team has followed this recommendation and will now finalize the standard EXAFS endstation while the

EXAFS spectrometer endstation has been lowered in priority. When up and running the beamline will serve many users requiring EXAFS. The beamline currently lacks a radiation safety permit to become operational. According to the plans presented to SAC the application was submitted at the end of June.

The VERITAS beamline was not discussed during the last SAC meeting. SAC noted good progress for this beamline at the meeting in November 2017, though it is significantly delayed compared to original plans (about 2 years). SAC at that point supported the development of the RIXS set-up. Funding for a second branch is available, but SAC finds that one end station at a time should be prioritized given the currently available resources. VERITAS plans for expert users at the beginning of 2019 and ramp up of regular user operation from fall 2019. Several other high-resolution soft-X-ray RIXS spectrometers are currently coming online worldwide with similar characteristics and delays at VERITAS may pose a risk in attracting the cutting-edge user community.

3.1.3 Beamlines under construction

Six beamlines are currently at different stages of construction; SPECIES, FlexPES MAXPEEM, SoftiMAX, CoSAXS and DanMAX. In addition, two beamlines, ForMAX and MicroMAX, have been recently funded.

SPECIES, FlexPES and MAXPEEM are beamlines that have been moved from the old MAX II ring to the 1.5 GeV ring at MAX IV. These beamlines are all awaiting radiation permits. As they are rather similar with respect to beamline construction, it is expected that once one of these three beamlines is approved the other two will also be approved rather quickly. Once radiation permits are given these beamlines are ready for commissioning. SPECIES is a versatile beamline covering several spectroscopic techniques, RIXS, NEXAFS, XPS and XAS as well as near ambient pressure XPS, the latter with strong links to the research performed at HIPPIE. FlexPES is another spectroscopy beamline serving the strong photoelectron spectroscopy community, while MAXPEEM provides world class aberration corrected spectroscopic photoemission and low energy electron microscopy.

The DanMAX beamline, funded by Denmark, has not been discussed by SAC except for its scientific profile. Thus, its progress and profile are not commented on.

SoftiMAX and CoSAXS are both in the phase where the beamline itself is under installation. Both beamlines are significantly delayed compared to original plans due to knock-on effects of delays at other beamlines and needed adjustments in priorities made by the MAX IV management. Based on advice from experts and potential users the SoftiMAX team has made some specific choices for the design of the STXM endstation, focusing on the STXM/ptychography endstation. SAC is very happy about the development and scientific choices made at this beamline. The progress of the CoSAXS beamline was not discussed during the last SAC meeting. This beamline will become a state-of-the-art small angle X-ray scattering (SAXS) instrument when operational.

ForMAX, funded in 2017, will serve as a versatile beamline for academic and industrial users, The beamline will in particular be directed to studies of wood-based materials and soft matter, and provide structural characterization from macroscopic to atomic level by combining X-ray imaging with small- and wide-angle X-ray scattering (SAXS and WAXS) along with X-ray imaging.

MicroMAX has been recently funded and will expand the MX portfolio at MAX IV. This beamline will take advantage of the properties of the MAX IV ring to deliver very small beams for microcrystallography. SAC is very pleased to see that the BioMAX and MicroMAX teams are working closely together. This will greatly facilitate the MicroMAX development, as well as allow both teams to support users in doing the right experiment on the right beamline.

3.2 General comments on the beamline development

At the SAC meeting in June 7-8 2018, it was evident that significant progress has been made over the last months with respect to reaching user operation at several beamlines. Short term planning of critical resources imposed by the management along with giving selected beamlines priority has contributed to this progress. It should also be noted that the MAX IV staff have made tremendous efforts to reach this point. This means that the facility now should be in a better position for producing scientific results, and indeed first user publications are beginning to appear.

However, as stated above, the beamline development at MAX IV is delayed for most of the beamlines. A priority of the laboratory should be to bring the 8 beamlines that were funded as the 1st phase beamlines into user operation. Some of these are now delayed by more than two years. The management have pointed out to SAC a number of issues causing this situation, some within and some outside the control of the laboratory. The funding situation before 2017 and the time required to hire the right staff are both elements in this picture. Building 16 beamlines, to large extent in parallel, is extremely challenging. In particular, common resources such as KITS need to be carefully planned. SAC finds that the situation in this respect has improved over time, however, KITS resources still appear to delay some progress in the laboratory. The most significant bottleneck at this point is the lack of radiation safety permits. SAC has recommended that MAX IV "immediately seeks to recruit additional staff, or secures support from peer facilities, to get radiation safety permits issued as soon as possible", as this is a critical issue for the progress at present. The MAX IV management has informed SAC that collaborations with other facilities are already in place to help this situation and that personnel has been recruited to ensure that this issue is now solved, see Appendix 4. A schedule for submission of applications for radiation safety permits has been made and submitted to VR, see Appendix 5.

Both MAC and SAC have pushed the 24/7 operation issue as this is critical for the operation of the facility and are happy that this is now in place. Now the agreements on user support need to be settled to avoid jeopardizing the user operation of beamlines.

Another very important request from MAC and SAC is to have access to a resources loaded schedule for the facility operation and development. The current time tables are provided at a too superficial level to serve as a useful planning tool on which SAC/MAC can give feedback. The short-term planning scheme introduced has been important for the recent progress but is not appropriate for a sustainable long-term planning of the laboratory. MAX IV has now entered a phase where user operations, commissioning and construction activities will run in parallel, making clear planning mandatory, including clear milestones. As stated in the SAC report: "Such milestones are, e.g., installation of the insertion device, first light in experimental hutch, installation of sample chamber, first user, etc. Such a plan, on a beamline **and** endstation basis, should also include indications of potential delays, estimates of the required man-power and other resources. It should also make clear, for the near- and mid-term, how relative beamline priorities will be adjusted and accompanying consequences

handled if delays occur." The MAX IV management has responded to this recommendation (Appendix 4): "At the June SAC meeting there was not enough time to present all the details of the operational planning which is already underway. The Pooled Resources Coordination Committee (PRCC) has made a prioritized list of the task for beamline, accelerator and infrastructure projects that identifies the resources required. Making this more detailed and connecting it to the timeline, with milestones for commissioning through user operations, is presently ongoing."

Finally, it should be pointed out that the next couple of years represent a window of opportunity for MAX IV as a unique diffraction limited source. Currently, several synchrotron facility development programmes towards diffraction limited sources are under implementation or in planning, including the ESRF upgrade programme. ESRF will close down in December 2018 for 20 months. After the upgrade, ESRF will become an extremely bright source with four new state-of-the-art beamlines fully exploiting the brilliance and coherence of the upgraded light source in addition to the already upgraded beamline program, presenting strong competition for MAX IV.