

# **Scientific case and beamline program**

## **Revised 20 Cell Design and the Conceptual Design Report of MAX IV**

### ***INTRODUCTION***

The *Science at MAX IV workshop*, held at Star Hotel in Lund the 29-31 October 2007, highlighted the user interest for beamlines in the hard X-ray regime. This in combination with the realization that several soft X-ray beamlines actually benefited from being placed on the suggested 3.0 GeV ring instead of the 1.5 GeV one, has made the relationship on the demand of beamlines on the suggested two rings somewhat less balanced. In the earlier design, reported in the *Conceptual Design Report of MAX IV* (CDR), two 12 cell lattice rings with a circumference of 287 meters were placed upon each other. In the new revised design a larger (530 meters circumference) 20 cell ring is planned and an upgraded MAX II ring is moved to the MAX IV facility. The latter ring will then mainly serve the soft X-ray community. The new design is an attempt to better reflect the demand of beamlines and to offer improved performances in especially the hard X-ray regime. In this document we try to make a summary of new experimental techniques/ beamlines that were discussed at the MAX IV workshop. We will report on the improved conditions with the revised design to offer competitive beamlines in especially the hard X-ray region. We also consider the consequences for the soft X-ray activities with the revised proposal.

### ***THE MACHINE***

#### ***Properties for the revised ring design***

The revised proposal entails building a larger 3.0 GeV ring with 20 cells in the lattice, and a lower horizontal emittance than for the original design of the 3.0 GeV ring. The 1.5 GeV ring of the CDR would be replaced by the MAX II ring, which is moved to new facility. Since there will be no need to cover the hard X-ray range with MAX II, it can be considered to lower the energy of the stored electrons in the MAX II ring from today's 1.5 GeV. In both proposals, the MAX III ring will be moved to the new facility, meaning that the situation is unchanged for activities on this ring. The table below summarizes the known properties of the two different designs for the 3.0 GeV and the 1.5 (or lower) GeV rings. The 12-lattice rings are those presented in the CDR report while the 20-lattice ring is the revised design.

Table I. Beam parameters of the storage rings

	Energy	Stored current	Horizontal emittance (nmrad)	Vertical emittance (nmrad)	Horizontal size (Sigma)	Vertical size (Sigma)
MAX IV 12-lattice	3.0 GeV	0.5 A	0.86	0.0086	83 $\mu\text{m}$	4 $\mu\text{m}$
MAX IV 12-lattice	1.5 GeV	0.5 A	0.34	0.034	52 $\mu\text{m}$	8 $\mu\text{m}$
MAX IV 20-lattice	3.0 GeV	0.5 A	0.24	0.009	44 $\mu\text{m}$	2.6 $\mu\text{m}$
MAX II original	1.5 GeV	0.3 A (max.)	8.8	0.9	350 $\mu\text{m}$	35 $\mu\text{m}$
MAX II upgraded	1.5 GeV	0.3 A	8.8	0.09	350 $\mu\text{m}$	16 $\mu\text{m}$
MAX II upgraded	1.0 GeV	0.5 A	4.5	0.05	280 $\mu\text{m}$	8 $\mu\text{m}$

### *The Emittance*

The horizontal emittance on the revised 20 cell ring would decrease to 0.24 nmrad for the 3.0 GeV ring. Already in the previous design, the emittance (0.86 nmrad) was outstanding compared to most other existing or planned sources. The vertical emittance is chosen by the coupling to match the diffraction limit at 1 Ångström, 0.009 nmrad. This was also the case with the previous design. With the revised design, the goals for the spot sizes reported in the CDR could be obtained with shorter beamlines, thus reducing the sensitivity for vibrations. The decreased emittance could also be used to even further decrease the spot size where that would be an advantage, i.e. the nanofocus beamlines. It must, however, be noted that to fully exploit the lower emittance, more severe demands must be implemented on the beamline optics (surface roughness and other errors). With the lowered emittance, also the coherent properties of the X-ray radiation are increased (see below). The vertical emittance on the upgraded MAX II ring can be expected to be lower than today, due to the smaller coupling allowed by full energy injection and top-up operation. Here, an energy of 1.0 GeV is considered, but the overlap with MAX III, with the energy 0.7 GeV, may motivate a different choice. On an upgraded MAX II ring, where the ring energy has been reduced to 1.0 GeV the horizontal emittance would decrease considerably. The lower energy would also allow running with 500 mA stored current, using the same amount of RF power, in particular as the two power consuming superconducting wigglers (I811 and I911) would not be installed on the moved ring.

### *The straight sections*

The length of the 20 (long) straight sections would be 5 meters. Out of these 20 sections, 19 can be used for insertion devices, and two of these sections should house superconducting multipole wigglers for optimal performance of the storage ring. With these wigglers, photon energies up towards 100 keV would be reached. The other straight sections would then have the same type of undulators discussed in the CDR, although the increase in length (from 4.6 m) will permit adding a few magnetic periods. Elliptically polarized undulators (EPU)'s covering energies between of 150

eV to 1.5 keV by the fundamental harmonic are the preferred insertion device for Soft X-ray spectroscopy beamlines to be placed on the 3.0 GeV ring. Different types of in-vacuum undulators would be the choice for the other beamlines, where energies up to around 30 keV would be reached.

### *The short straight sections*

There are 2 short straight sections per cell in the 20-cell lattice, which gives a total of 40 short straight sections in the ring. 10 of these 40 short straight sections will be used for RF cavities and another 2 for injection kickers. There is hence up to 28 short straight sections available for the installation of insertion devices for the production of synchrotron radiation. The length of a short straight section is 1.47 m measured magnet to magnet. It is estimated that insertion devices with a magnetic length of approximately 1 m can be installed in the short straight sections. The length of the short straight section is too short for the installation of undulators but there is sufficient length for multi pole wigglers or wavelength shifters. The influence from wigglers and wavelength shifters installed at the short straight section on the dynamic aperture of the storage ring requires further study. The expected flux of photons can however be estimated by assuming a 24 pole wiggler with a peak field of 1.8 T and a period length of 8 cm. The magnetic gap of such a device is 12 mm. The expected flux of photons in the energy range 100 eV - 50 keV is shown in the figure below.

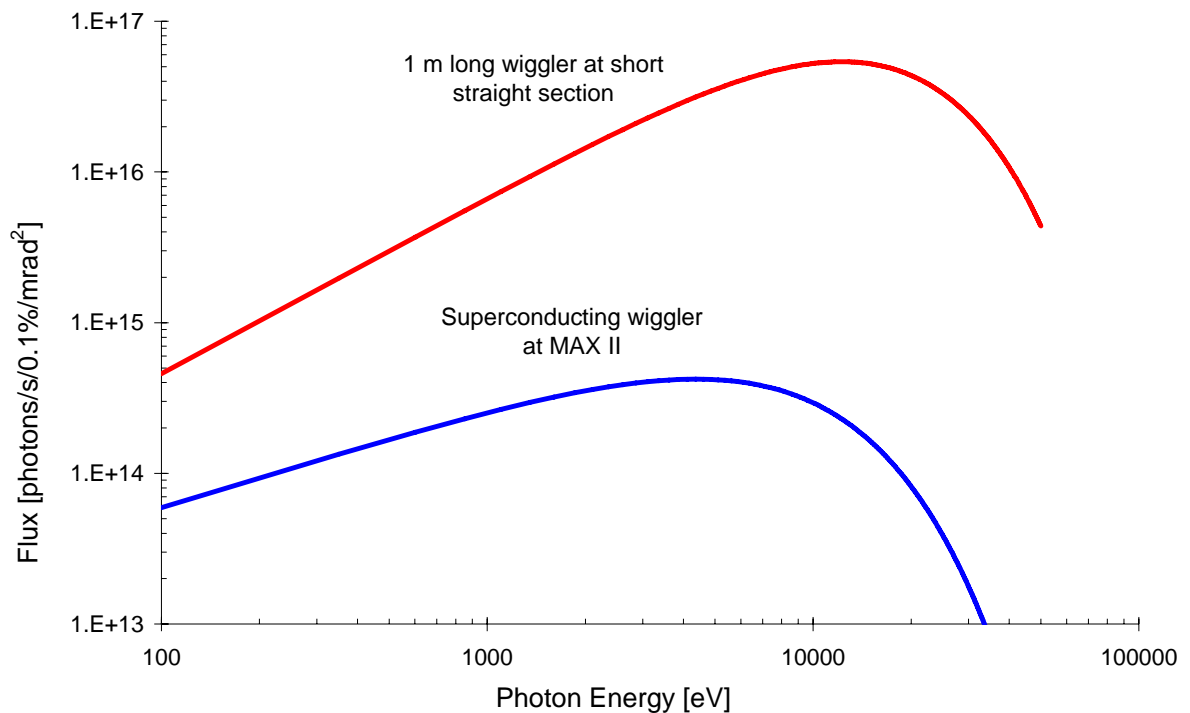


Figure 1. Calculated flux for a 1 m-wiggler at the 3.0 GeV ring at MAX IV, compared to the present superconducting wigglers at MAX II

## **CONSEQUENCES FOR HARD X-RAY ACTIVITIES**

### ***Beamlines at the 3.0 GeV ring in the CDR report.***

In the *MAX IV Conceptual Design Report* from 2006, the number of possible beamlines on the 3.0 GeV ring was limited to eleven, nine very high performance undulator and two high energy/high flux wiggler beamlines. The design does not permit using the bending magnets as radiation sources for the hard X-ray beamlines. In the report the following beamlines were suggested to be housed at the 3.0 GeV ring:

- Nanofocussing: Microscopy and Spectroscopy (NANO-1)
- Nanofocussing: Diffraction, Imaging and  $\mu$ -tomography (NANO-2)
- Macromolecular Crystallography: High-throughput and Phasing (MX-1)
- Macromolecular Crystallography: Microfocus (MX-2)
- High Resolution Powder Diffraction and Small/Wide Angle X-ray Scattering
- Microfocus X-ray Spectroscopy
- Very High Resolution Soft X-ray Spectroscopy
- Magnetism: Spectroscopy and Spectromicroscopy
- Materials Science and Extreme Sample Conditions (wiggler)

With this suggestion, nine out of eleven possible straight sections would be occupied already from the beginning, and only one of the remaining straight sections could be used for an optimized undulator, as one of them would have to house the second wiggler. This would be a serious limitation on the possibility of future expansion into other experimental techniques, not presented in this proposal and limit the possibility to relocate existing beamlines on the MAX II ring to the 3.0 GeV ring where they could still serve an important purpose, *e.g.* I811 and I911. The limitation in the number of possible beamlines has also put some pressure on sharing different experimental techniques onto the same beamline in ways that would be suboptimal.

### ***Suggested beamlines/ experimental techniques at the 3 GeV ring that are not present in the CDR:***

At the *Science at MAX IV workshop* several suggestions for new beamlines and new experimental techniques that are not present in the CDR were discussed.

#### ***A dedicated SAXS beamline***

SAXS is, especially at MAX-lab, a rapidly expanding experimental technique and a special and well attended session on the subject was organized during the Science at MAX IV workshop. Several participants expressed concern that sharing the two experimental techniques of powder diffraction and SAXS, as suggested in the original CDR report, is not an optimal solution. Even though the suggested design would not result in sacrificing the performance, the fact that two separate techniques are implemented on the same beamline inevitably results in a loss of beamtime when changing between the techniques. The expanding activity within this field may also suggest that a dedicated SAXS beamline may better reflect the need within this user community. Another very attractive possibility would be to be able to offer a dedicated set-up for micro fluidic cell measurements. Considerable work is put into the technique of micro fluidic studies within the user community interested in macromolecular solution scattering (bioSAXS). Micro fluidic studies permit using

very small volumes, thus for instance enabling scanning over a wide range of different sample environments, in terms of e.g. salt concentration or pH, to find the optimal crystallization conditions or to study reactions involving macromolecules in physical relevant conditions. The technique has proved to be very promising, and a collaboration with a very active user group at Copenhagen University within this field has resulted in successful measurements at the rather restricted set-up on beamline I711. A dedicated station equipped with such a cell would be very attractive for a large and growing user community. Such a station could very well be placed on one of the short straight sections.

### ***Powder diffraction***

An interest in performing powder diffraction at higher energies than those that are obtainable at an undulator beamline on the 3.0 GeV ring ( $< 30$  keV) has indicated that such a beamline/ station could be placed on one of the wiggler stations. This would permit experiments with energies up towards 100 keV. The increased flux at a wiggler source will also make it, in combination with a fast position sensitive detector, very suitable for kinetic studies down towards the millisecond regime. However, the superior collimation of an undulator beam will make it the preferred choice for the most demanding experiments in terms of resolution. Experiments, like structural refinement of more complex substances, where an instrumental resolution of  $< 0.01^\circ$  is required, suggest a high resolution scanning powder diffractometer to be placed on a minimal (vertical) divergence X-ray beamline. Suggestions of combining the technique with different types of spectroscopy (i.e. XAFS and Raman) methods are also of interest.

### ***An Environmental Science beamline in the energy range of 1 – 3 keV***

The energy range of 1-3 keV is of special interest for the environmental science community as the absorption edges for aluminium, silicon, phosphorus and sulphur are in this region, elements of utmost importance in many environmental research areas. This energy regime is considered to be difficult since it is in the intermediate range between grating and crystal optics, but such a beamline on MAX IV should be able to benefit from recent experience in this field.

### ***Relocation of MAX II beamlines***

The relocation of beamline I811 and the central SAD/ MAD station on I911 is mentioned as a possibility in the design report. If these beamlines could be moved to the new facility without any major modifications they would offer a very cost effective possibility to do bulk experiments with EXAFS and protein crystallography. The limited number of straight sections and the limited possibility of using the bending magnets due to their inadequate spectral range would, however, make this unlikely. The revised 20-cell ring design with as many as 28 shorter (1.47 m) straight sections suitable for 1-meter long wigglers would match the requirements for these relocated beamlines very well.

### ***High kinetic energy photoemission***

In the CDR, the idea of building a high kinetic energy photoemission endstation at the Materials Science wiggler beamline was mentioned. However, the increasing involvement and interest from Swedish and Nordic groups in this technique motivate

a more dedicated solution. At the session concerned with high kinetic energy photoemission at the Science at MAX IV workshop it was made clear that an undulator source would be much superior to a wiggler for this purpose, and that the combination of photoemission with scanning techniques such as EXAFS on the same beamline is impractical. Instead, a combination with inelastic X-ray scattering, a spectroscopic technique with similar demands, would be much more suitable.

### ***Beamlines for the exploitations of the coherent properties of the radiation***

The coherence of the radiation will increase from the lowered emittance of the redesigned 3 GeV ring, and this will be beneficial for some activities, such as spectroscopy and spectromicroscopy of magnetic samples (*e.g.* speckle spectroscopy). Additionally, the exceptionally small emittance of the 3.0 GeV ring makes it an ideal source for X-ray photon correlation spectroscopy (XPCS). This possibility was not pointed out in the CDR, but a session at the Science at MAX IV workshop demonstrated the growing interest in the XPCS technique. The prospect of offering such capabilities at MAX IV should therefore be kept in mind.

### ***CONSEQUENCES FOR SOFT X-RAY ACTIVITIES***

A change in the conceptual design of the MAX IV facility will affect soft X-ray research more profoundly than the hard X-ray activities. Below, some specifics for the beamlines and activities presented in the CDR will be discussed, but some general observations can be made. An upgraded MAX II storage ring can partly cover the needs for the soft X-ray communities, if a dedicated new 1.5 GeV ring is not built. One drawback of such a solution is that the straight sections in MAX II are shorter than those originally planned for MAX IV (3.2 m vs. 4.6 m), and do not allow the same number of periods of the insertion devices for the same energy, meaning that the flux will be lower. With the new linac injector, full energy injection will become possible for the MAX II storage ring. This will allow top-up operation<sup>1</sup>, which will increase the average current, even if it will not be as high as in the original MAX IV design (0.3 A vs. 0.5 A). Since the beam lifetime becomes irrelevant for top-up operation, the coupling between horizontal and vertical beam size can be decreased. The vertical emittance can then be decreased substantially, improving the beam quality to such a level that the contribution from the source size on the photon energy resolution is negligible for entrance slit-less grating monochromators, *e.g.* SX-700 type PGMs and collimated PGMs. However, neither the brilliance nor the flux will be on par with that achievable at the originally proposed 1.5 GeV ring.

If the soft X-ray beamlines were instead located on the new 3.0 GeV ring, their performance would be equal or better than at the optimized 1.5 GeV ring for photon energies above the C 1s edge ( $\approx 300$  eV). A large part of the soft X-ray activities would have an improved situation at the higher energy ring, especially as the horizontal emittance for the 20-lattice 3.0 GeV ring is even lower than for the 12-lattice 1.5 GeV ring. However, there are important energy ranges below the C 1s edge, *e.g.* the Si 2p edge, the actinide 4d edges and the 3p edges of the 3d transition metals, where a high performance is crucial for many user communities. For these energies, a possible way of improving the performance of MAX II, is to lower the

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<sup>1</sup> Issues concerning heat load and radiation need to be investigated further.

energy of the storage ring. Lowering the energy from 1.5 GeV to 1.0 GeV will first of all decrease the horizontal emittance. Secondly, by decreasing the period length of insertion devices, which will shift the energy spectrum to shorter wavelengths, and by increasing the number of periods for the same device length, a higher flux can also be obtained<sup>2</sup>. With an undulator period of 2.5 cm and a device length of 2.5 m, the brilliance at 1.5 keV will be in the  $10^{18}$  ph/(s 0.1% BW mm<sup>2</sup> mrad<sup>2</sup>) for 1.0 GeV operation, comparing favorably with today's situation at MAX II. The lowered energy also means that a higher current may be stored in the ring, even using the same vacuum and RF power system as for the present MAX II storage ring.

### ***Specific beamlines***

In the CDR, four beamlines intended to be built at the 1.5 GeV ring were presented:

- 1) Ultra high resolution VUV scattering
- 2) Soft X-ray nanoscience and spectromicroscopy
- 3) Soft X-ray spectroscopy and surface reactions
- 4) Soft X-ray gas phase spectroscopy

Additionally, the possibility of relocating the beamlines I311, I411, I511 and D1011 to the new ring was considered. Some of the more salient points for each beamline with regards to the situation at MAX IV are discussed below.

#### *1) Ultra high resolution VUV scattering (30-600 eV)*

VUV scattering is a very flux demanding experiment. The achievable resolution depends very much on the spot size at the sample position, and the design goal for the spot size in the CDR was 1x1  $\mu\text{m}$ . This beamline is similar to one suggested for the 3.0 GeV ring (the *Very High Resolution Soft X-ray Spectroscopy* beamline), but working at a lower energy. For that reason, transfer to the 3.0 GeV ring is not an option. At an upgraded MAX II, this beamline will benefit from a lowered energy of the storage ring, since the reduced horizontal source size will simplify focusing to the desired spot size. The possibility of increased flux from a higher current and more periods of insertion devices for the 1.0 GeV solution would also be an advantage.

#### *2) Soft X-ray nanoscience and spectromicroscopy (90 -1500 eV)*

Similar considerations apply to this beamline as to the *Ultra high resolution VUV scattering* beamline: A small spot size is needed on the sample, for both the X-PEEM and the STXM endstations. If this beamline were instead placed at the 3.0 GeV ring, the spot size demand can be met, but the whole desired energy range will not be covered. A second beamline may then have to be built at the lower energy ring to cover the lower energy range. For the lower energy range, it would benefit from a lowered energy of the storage ring, to obtain a smaller focus and to increase flux. The user demand may well be enough to motivate two beamlines.

#### *3) Soft X-ray spectroscopy and surface reactions (60-1500 eV) and*

#### *4) Soft X-ray gas phase spectroscopy (90-1500 eV)*

These beamlines have more moderate demands on the beam size at the sample than the two previous beamlines. Since the full energy range can be covered by optimized undulators at MAX II, operating at 1.0 GeV, and the lowered vertical emittance will allow very high photon energy resolution, so the prospect of building these two beamlines on MAX II will mean only minor drawbacks. An alternative approach

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<sup>2</sup> This will depend on the K-value of the insertion device.

could be to build these beamlines at the 3.0 GeV ring, which would give an even better performance above the C 1s edge than in the original proposal, and to let the lower energy range be covered by relocated MAX II beamlines (I511 and I411, respectively), on the 1.0 GeV ring.

## ***CONCLUSIONS***

The new 20-cell lattice design will give an improved situation for all hard X-ray activities, and also for the soft X-ray activities presented in the CDR, which were intended for the 3.0 GeV ring. The larger number of straight sections will allow more freedom to build new beamlines in the future, as is motivated by technological development and on user needs. The prospect of putting insertion devices in the short straight sections, which will give additional possibilities of new beamlines, was not accessible in the original design. Finally, the decreased horizontal emittance will improve the performance, giving a higher brilliance to an already outstanding source.

The new concept will offer very impressive performance also in the soft X-ray range. For two of the suggested beamlines (the surface reactions beamline and the gas phase beamline), the performance at an upgraded MAX II ring will be very close to the goals in the CDR. There is also the option of building the beamlines at the 3.0 GeV ring, and letting the lower photon energy range be covered by relocated beamlines from MAX II. For the other two (the VUV scattering beamline and the soft X-ray microscopy beamline), the emittance of an upgraded MAX II ring will not give the same possibilities of focusing the radiation to a small spot on the sample as the original proposal. For the soft X-ray microscopy beamline, there is the option of building the beamline at the 3.0 GeV ring, which would give equal or superior performance above the C 1s edge.