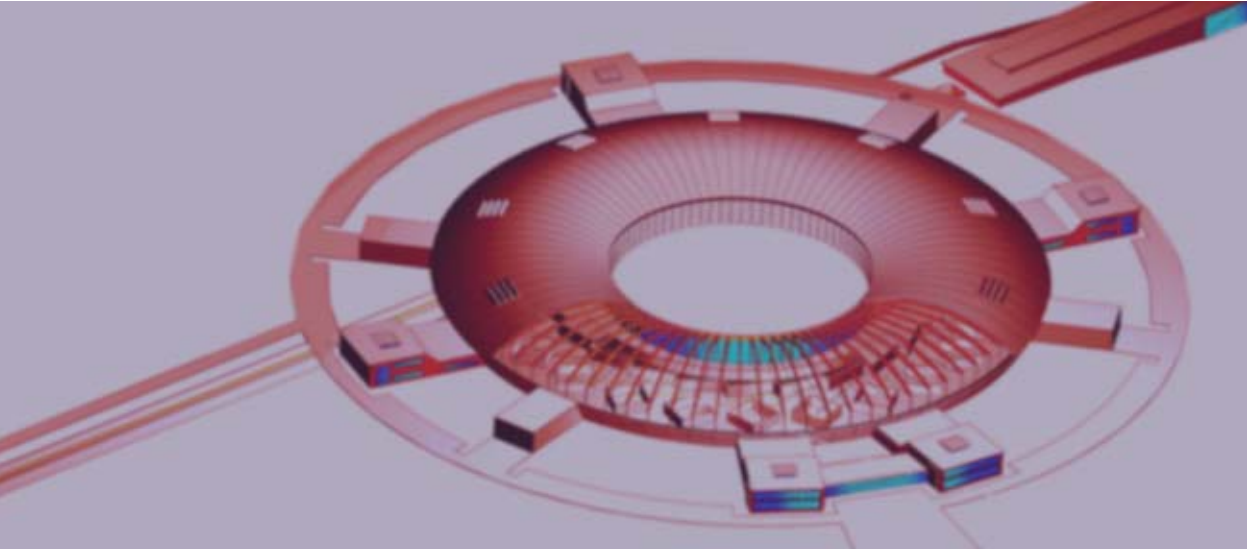




Vetenskapsrådet



SCIENTIFIC EVALUATION OF THE MAX IV PROPOSAL



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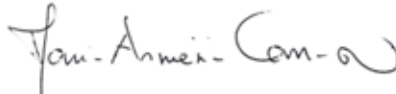
The Committee for Research Infrastructures (KFI) at the Swedish Research Council (VR) decided in early 2005 to evaluate the technical and scientific case of a proposal by the MAX Laboratory in Lund for a new synchrotron radiation facility named MAX IV. For the evaluation of the scientific case a panel of international experts was appointed with a Swedish chairperson as well as a Swedish secretary. The expert panel visited MAX-lab on 19-20 October, 2006.

The present document reports the assessments of the expert panel. By signing, the international experts take full responsibility for the report. The chairperson and the secretary confirm that the work was conducted in accordance with the statutes of the Swedish Research Council and that it was performed in an impartial manner.

November, 2006



Prof. Yvan Bruynseraede



Prof. Maria Arménia Carrondo



Prof. Wolfgang Eberhardt



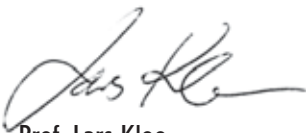
Prof. Michael Grunze



Prof. Britt Hedman



Prof. Chi-Chang Kao



Prof. Lars Kloo

Chairperson



Dr. Per Karlsson

Secretary

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SUMMARY

This is a report on the scientific case for a future MAX IV synchrotron radiation facility at Lund University. The plans for MAX IV include two new storage rings at 1.5 and 3.0 GeV, respectively, and the transfer of an existing 0.7 GeV storage ring. The possibility for the use of a free electron laser (FEL) is taken into account by designing the facility with a 3 GeV linear accelerator (Linac).

The Evaluation Panel has considered both the scientific opportunities presented in the “2005 MAX IV Conceptual Design Report” and the presentations made at a hearing at MAX-lab in Lund, October 2006. The innovative and cost-effective design presented by the MAX-lab team, building on the experiences made in the construction of existing MAX-lab synchrotron rings, offers possibilities for a world-leading and unique light source. In particular, the high brilliance, the high flux of the storage rings and the ultrafast capability provided by the Linac will allow a unique combination of having spatial resolution into the nanometer range and the study of dynamics into the femtosecond regime.

The Evaluation Panel is unanimous in its conclusion that the scientific case for a MAX IV facility is very strong, representing a site for intrascientific challenges as well as interscientific advances and an important resource for upgraded industrial research in the Nordic and possibly Baltic countries. The Evaluation Panel is clear in its recommendation to the Swedish Research Council:

MAX IV should be funded to the level requested, and the funding should commence as soon as possible.

PROCEDURE FOR THE EVALUATION

In May 2005 the MAX-lab in Lund submitted a proposal to the Swedish Research Council (VR) for the funding of a Detailed Design Study for a new synchrotron radiation facility named MAX IV. In the proposal there was a request for 28 MSEK for this study. The Committee for Research Infrastructures (KFI) at the Council processed the proposal and decided in November 2005 to fund the proposal with 4 MSEK for 2006. In order for the proposal to qualify for further funding the Committee decided that the technical and scientific case for MAX IV must be evaluated. The Committee appointed an Evaluation Panel to scrutinize the scientific case. The instructions given to the Evaluation Panel are summarized as Terms of Reference in Appendix 1. Prof. Lars Kloo, at the division for Inorganic Chemistry at the Royal Institute of Technology in Stockholm, was appointed chairperson of the Panel with Dr. Per Karlsson from the KFI staff as secretary.

The international expert members of the Evaluation Panel were:

Prof. Yvan Bruynseraede, K.U.Leuven, Belgium

Prof. Maria Arménia Carrondo, Universidade Nova de Lisboa, Portugal

Prof. Wolfgang Eberhardt, BESSY, Berlin, Germany

Prof. Michael Grunze, Heidelberg, Germany

Prof. Britt Hedman, SSRL, Stanford, USA

Prof. Chi-Chang Kao, NSLS, Brookhaven, USA

Short CV's for the Panel experts can be found in Appendix 2.

The Evaluation Panel visited the MAX-lab on October 19-20, 2006. The first day of the visit included general presentations by representatives from MAX-lab, Lund University and the City of Lund, as well as a selection of scientific seminars by the MAX-lab user community. On the second day the Panel discussed a preliminary version of the report and had a short meeting with the MAX-lab management for questions. The Agenda of the visit is included in Appendix 3.

Before the site visit the Panel received documentation about the project: "2005 MAX IV Conceptual Design Report" (CDR), MAX-lab Activity Report 2004 and a cost estimate of MAX IV (Appendix 4), as well as Terms of Reference (Appendix 1), and previous evaluations of national facilities in Sweden (2002) and the MAX IV technical concept (2006).

EVALUATION OF THE SCIENTIFIC CASE

Introduction

Synchrotron-based research has moved from being a challenge within accelerator physics alone to becoming a versatile and widespread scientific tool. Today, a state-of-the-art light source attracts a broad range of scientific communities with the unique experiments that can be performed at synchrotron radiation sources. The driving forces of development represent a unique symbiosis between accelerator design and the ultimate user demands on the resulting synchrotron radiation.

The 4th generation facility in the present MAX IV proposal, through its high brilliance, will allow experiments probing structural and physical phenomena at nanometer scale spatially and the evolution of fast dynamic processes at femtosecond scale temporally. Thus, fundamental insights will be obtained to the benefit of a wide range of scientific disciplines. The new facility will also have great impact on interdisciplinary research, industrial research and education/training of the next generation of scientists and engineers.

The evaluation of the scientific case for a MAX IV facility has been based on both the “2005 MAX IV Conceptual Design Report” (CDR) and a hearing at the MAX-lab in Lund, October 2006. In the CDR the scientific opportunities are divided into 13 different areas, many of which are interdisciplinary with respect to the traditional subjects within the natural sciences. For practical reasons these can be merged into larger sections, as presented in the evaluation below.

In each section, comments guided by the Terms of Reference (Appendix 1) are given. More specifically, the most important experiments that can be performed at a future MAX IV facility are highlighted, the relevance of the choice of ring energies and beamlines is commented upon, and the uniqueness and realism of proposed goals and potentially overlooked experiments are brought forward.

Life science & protein crystallography

Macromolecular crystallography

Synchrotron radiation-based macromolecular crystallography has revolutionized the ability to determine the structure of biomolecules, such as large

macromolecular complexes, which are essential to the understanding of life processes, and therefore has had an immense impact on central areas in biology. Examples are the structures of the ribosome itself as well as complexed with small molecules, which are the largest particles ever crystallized; and RNA polymerase in complex with DNA at various stages in its functional processes, a study which was awarded the 2006 Nobel Prize in Chemistry.

The proposed science in this area is addressing the understanding of function of macromolecules by determination of their structures. The specific types of problems targeted include large macromolecular complexes, membrane proteins, viruses and viral proteins, time-resolved studies of reaction mechanism in enzymes, and – when possible – structure determination at atomic resolution ($<1 \text{ \AA}$). All described areas are highly important in molecular biology and medicine. For example, it is estimated that 50% of the targets for current medical drugs are membrane proteins, yet the number of membrane protein structures in the Protein Data Bank (PDB) is very low as compared to non-membrane proteins. Even structural genomics efforts have not yet begun to overcome this problem. Another important area is that of drug design, where for example the issue of antibiotic resistance requires knowledge of how new antibiotic drugs interact with large complexes, like ribosomes.

There are also many other important areas of structural biology that address biomedical or biological questions, for which the ability to perform the measurements rapidly on larger crystals can be equally important. This includes industrially based drug design projects, which (just like the weakly diffracting systems described above) require the automated screening of hundreds of crystals. Structural biology and targeted scientific biological and biomedical projects are growing with the current strong expansion of macromolecular crystallography groups in the Nordic countries.

The synchrotron design for the 3 GeV ring will provide a source that is of ultra-low diffraction-limited emittance, and high current in top-off mode, with world-leading brilliance and flux. It is ideal for macromolecular crystallography and excellently meets the requirements of the proposed science.

Two MX beamlines are proposed, one optimized for high throughput and phasing based on anomalous scattering (MAD and SAD), which will have highly parallel beams with a $\sim 60 \times 30 \text{ \mu m}$ focus at the sample. The second beamline is a microfocus tunable beamline, especially adapted for studies of large unit-cell and/or weakly diffracting crystals, which are typical for large molecular assemblies and membrane protein crystals. It is particularly suitable for microcrystals with a beam size at the sample of $\sim 10 \times 7 \text{ \mu m}$, with very high brilliance and required stability.

Few macromolecular crystallography beamlines world-wide are truly unique, due to the implementation of a large number of stations driven by the

very extensive user community. However, the proposed beamlines will be state-of-the-art and internationally entirely competitive. Currently, there are very few microfocus beamlines operational or in construction/planned with the world-class brilliance and small beam size proposed for the MAX IV beamline, which will provide outstanding performance.

Small-angle X-ray scattering

Biological solution small-angle X-ray scattering (SAXS) allows direct study of the size, shape and dynamics of biological molecules under functional biochemical conditions. It is also used for the study of the various steps in complex formation, and for obtaining information relevant to crystallization processes. It bridges between macromolecular crystallography and electron microscopy, and provides unique biological information. Small-angle diffraction is used for fiber and muscle studies. It is a growing field as it is increasingly combined with crystallographic studies, and its use for structural genomics is being realized. The scientific questions proposed for study at MAX IV are highly relevant to structural biology and biomedical applications. Using ultra-small volumes and high-brilliance beams, the method will be used for time-resolved studies at the ms to μ s level. The method is important also for pharmaceutical industry to monitor the status of engineered proteins and drug delivery processes. There is a growing community in the Nordic countries that is forming a strong center, competitive world-wide, and their proposed studies in structural biology for basic understanding of structures in solution and for direct biomedical problems are strong.

The synchrotron design for the 3 GeV ring will provide a source that is of ultra-low diffraction-limited emittance, and high current in top-off mode, with world-leading brilliance and flux. It is ideal for the proposed studies and meets the requirements of the proposed science.

One beamline is proposed (shared with powder diffraction) and its optics has been defined to provide a high-brilliance, very small beam that meets the requirements for minimal sample consumption. Automation is planned, and the characteristics of the beamline match the experimental requirements well.

There are several small-angle scattering beamlines at other synchrotrons but very few optimized and dedicated for biological SAXS. The proposed beamline will be state-of-the-art and internationally very competitive. However, its additional function of providing a facility for powder diffraction needs to be addressed in the design phase so that its SAXS performance is not compromised.

Materials science

This section addresses condensed matter physics and materials science, in particular strongly correlated electron systems, magnetism, soft and biological materials, and materials research in industrial applications.

The understanding of strongly correlated electron systems, with high-temperature superconductivity being the most well-known example, is one of the most important problems in condensed matter physics today. The proposed experiments, high-energy and micro-beam photoemission spectroscopy, resonant elastic and inelastic X-ray scattering, are all identified in a recent “Basic Energy Sciences Workshop Report: Basic Research Needs for Superconductivity” sponsored by the U.S. Department of Energy. They are the emerging experimental techniques that, in combination with other more established experimental techniques, will allow for the first time the complete determination of all relevant electronic and magnetic structures of high-temperature superconductors.

The most important current problems in magnetism and magnetic materials development are the understanding of interfacial magnetism, switching dynamics and molecular magnets. The combination of high-brilliance storage rings and the ultra-fast capability provided by the Linac is ideally suited to study these problems. The proposed sub-10 nm magnetic imaging, the high-energy as well as high-resolution angle resolved photoemission, resonant magnetic scattering, and sub-picosecond time-resolved pump-probe capability proposed are all identified in a recent review of “Advances in Nanomagnetism via X-ray Techniques” (Journal of Magnetism and Magnetic Materials, December 2006) as very desirable experimental tools.

In the soft and biomaterials area, the scientific areas identified in the CDR – organic electronics and bioelectronics; organic spintronics; molecular switching for memory technology; molecularly modified surfaces and interfaces; biomaterials; polymers; biocompatible nanoparticles; self-assembled structures, micro- and nano-arrays – are all areas of current interest. In particular, the study of ultra-fast processes in charge transfer, molecular switching, and interfacial processes is clearly at the cutting edge and the unique capabilities provided by MAX IV will be essential.

The use of synchrotron radiation to address industrial problems is growing rapidly world-wide. The proposed high-resolution three-dimensional X-ray diffraction tomography as well as *in-situ* studies of material processing and chemical/electrochemical processes are all good uses of the sources. Another important point is that there is a strong and fairly large local and regional industrial interest in using the proposed MAX IV facility.

MAX IV will be a synchrotron source with world-leading brilliance and flux. The proposed experiments in materials science will be pushing the limits in energy and spatial resolution beyond those of current facilities. The proposed experiments take full advantage of the traditional strength of the Swedish research community in electron and X-ray spectroscopy as well as the world-class instrumentation development capabilities in these areas. For example, the soft X-ray resonant inelastic beamline, and the high-energy photoemission beamline and end-stations, will be unique in the world.

With a unique light source such as the MAX IV at hand, there are several areas that could be emphasized, and where the planned synchrotron facility could make a difference. Examples are:

- 1 The high brilliance of MAX IV is ideal for using coherent X-ray scattering in the study of equilibrium and non-equilibrium dynamics in both soft and hard condensed matter systems.
- 2 The high flux from MAX IV, a factor of 5-10 more than at the ESRF for photon energies between 8-10 keV, is extremely important for inelastic X-ray scattering. The gain in flux can be used to improve energy resolution of the experiments, for example on lattice dynamics in soft materials, or to study charge dynamics in higher-Z materials that cannot be studied today.
- 3 The high brilliance and flux of MAX IV are ideal for high-momentum-resolution resonant and non-resonant X-ray scattering study of phase transitions in strongly correlated and magnetic systems. This class of experiment is complementary to high-energy-resolution spectroscopic and high-spatial-resolution imaging experiments which are described in detail in the scientific case.
- 4 Facilities and infrastructure to support extreme experimental conditions, such as high magnetic field, low/high temperature and high pressure, should be included in the beamline planning.
- 5 The possibility of using the Linac for ultra-fast X-ray experiments is mentioned in a number of experiments. It would be useful to have these ideas developed fully to guide the design of the development of the ultra-fast beamline.
- 6 To take full advantage of the wide range of wavelength covered by MAX IV, it is important to consider how to integrate materials synthesis with experiments and the utilization of multiple experimental techniques.

Solids, surfaces, interfaces and nanoscience

The scientific questions have been identified by dedicated scientific panels and have been discussed thoroughly. The major fields and open questions

that are described in the CDR give a very good representation of up-to-date and challenging research lines that will directly benefit from the use of synchrotron radiation. Concerning the fields of nanoscience, nanotechnology, surfaces and interfaces, the following comments can be made.

The CDR addresses the important field of nanoscience and presents several strategies to perform ground-breaking work in that field (very small systems, very fast phenomena etc.). The topical field of nanoscience is growing exponentially and encompasses structures such as nanotubes, nanowires, new oxide materials, quantum dots, clusters, and other low-dimensional forms of matter. It opens new insights and possibilities in photonics, electronics, magnetism, metals and alloys, ceramics, and other areas. Progress in nanoscience and nanotechnology is also likely to have a large impact on reducing energy consumption, e.g. in catalytic processes and in energy storage devices. Nanomaterials have for instance revolutionized the science of catalysis by providing new methods for producing catalysts with more accessible surface area, and for controlling their crystallographic structure, size, shape, alloy content, and array organization. Many materials acquire new chemical properties at the nanoscale, related to the size-dependence of their electronic structure.

Nanostructures enable the production of materials exhibiting many new and desirable, technologically relevant properties not displayed by their bulk counterparts. Progress in nanomedicine, i.e. the control of biomolecular processes by nanosystems on a cellular level, for example, will depend on our ability to control and predict the biophysical and biochemical properties of nanoparticles. The design of nanoscale architectures with the required interpenetrating new properties represents fascinating challenges, in which upgraded synchrotron-based X-ray techniques and spectroscopies will play an important role. With respect to the CDR, we agree completely with the Swedish Science Council report "Evaluation of the Swedish Condensed Matter Physics, 2004" and quote: *"...nanoscience has become a major component of the activities of several research groups which had previously engaged in work in the related areas of surface and cluster physics. Indeed, high quality research in nanoscience is being carried out in varying extents in almost all universities in Sweden"*.

The role of the surface and interfaces between adjacent materials becomes increasingly relevant with decreasing size of the structural units. Self-assembly over several length scales, also referred to as a "bottom-up" approach in creating novel electronic and mechanical devices, depends on our ability to control surface and interface phenomena on the nanoscale. Moreover, new dynamic phenomena are expected in very small structures. Since the properties of surface structures are different from those of corresponding bulk materials, new methods have to be developed for their experimental characterization and modelling.

“At the nanoscale, interfaces are everything”. The ability to characterize buried interfaces at the atomic scale is the key to understanding them and developing better devices. The ultimate goal is to be able to image the ultra-fast movements of atoms at the interfaces – essentially creating a movie of atomic motion. The extremely high flux of X-rays produced by synchrotron storage rings makes it possible to probe layers and interfaces in complicated stacked structures by spectroscopy, characterize low-atomic-weight materials such as polymers, and study *in situ* phase transformations, to name only a few applications. The third-generation X-ray synchrotrons are a major step toward this ultimate goal. They produce a partially coherent, quasi-monochromatic X-ray beam with a brilliance that exceeds that of the previous generation by many orders of magnitude. The future Linac-based source will produce picosecond X-rays that will enable us to take snapshot ps images with atomic resolution for the first time. Particularly the application of new synchrotron radiation sources opens qualitatively novel perspectives for investigations of diffusion in surfaces, interfaces and near-surface layers. Again, using the words of the above-noted report we conclude that *“Surface science remains strong in Sweden; indeed, this is certainly one of the strongest areas of condensed matter physics in Sweden. In part this stems from the traditional strength in electron spectroscopy, and there is no doubt that some Swedish groups continue to play a leading role on the world stage in developing new and existing electron and related spectroscopies”*.

The CDR provides a very fair assessment of what quality of radiation can be expected from the synchrotron rings. The proposed synchrotron rings, covering the full electromagnetic spectrum needed in materials science and biology, will provide the brilliance and stability of radiation needed for the research. Time-resolved experiments will be of particular interest and importance. There are still a number of important decisions to be made concerning the precise technical details of the 1.5 GeV ring, but considering the experience of the design team, it is safe to expect that the remaining problems will be solved satisfactorily.

The proposed beamlines are state-of-the-art, in many respects complementary and more advanced compared to other installations, and will indeed be adequate for the proposed experiments. The Panel raises the question whether it would be possible to combine the beams with different energy within one experimental station.

The beamlines and experiments will compete with similar instruments at other European synchrotron facilities, which plan major upgrade programmes or which are presently under construction (PETRA III). However, the demand and need for highest-quality tools of characterization will also exceed the supply in the future.

The use of a 'double' ring (3 GeV and 1.5 GeV stacked on top of each other) is a unique and cost-effective solution. The presence of beamlines making use of an exceptionally broad range of the electromagnetic spectrum within a single facility is a unique and favourable association and provides a very interesting opportunity for fruitful exchanges between researchers and scientific disciplines that would otherwise make use of separate facilities. MAX IV will be a very important resource for the Nordic science community, but also for the international users. The opportunity to integrate very different scientific communities is certainly an asset and a strong argument in favour of the construction of a synchrotron facility in a relatively small country.

Recently, the European Commission published a report prepared by the Scientific Committee on Emerging and Newly Identified Health Risks (SCENIHR). This committee expressed an *"Opinion on the appropriateness of existing methodologies to assess the potential risks associated with engineered and adventitious products of nanotechnologies"*. It might be of interest to address the possibilities offered by MAX IV in risk assessment of nanotechnologies.

Spectroscopy of atoms and molecules

Atoms and molecules offer a seemingly simple testing ground for new concepts in spectroscopy and theory, leading to an improved understanding of electronic interactions and electronic structure. Relativistic effects in the electronic interactions are ideally studied by high-precision spectroscopy of atomic systems, which serves as the ultimate testing ground for improved theoretical concepts. The combination of the high-resolution advanced instrumentation for photoelectron spectroscopy or soft X-ray emission spectroscopy with the tunable high-resolution synchrotron source at MAX II has helped to develop a research community with world-wide recognition and an outstanding track record in this field. There are not only Swedish groups involved, but also groups from other Nordic countries, especially from Finland. They also have contributed to the investment in beamlines and instrumentation at MAX II, and the new source MAX IV will again lead to a quantum jump in resolution and overall performance for this field, which will be accompanied by the corresponding advance in basic scientific understanding of these seemingly simple systems.



EVALUATION OF THE UNIQUE MAX IV POSSIBILITIES

Ultra-fast phenomena

The combination of a synchrotron source jointly with a short-pulse Linac source, which can be expanded into an FEL facility, is unique in the design of the MAX IV project. The same Linac is being used in a highly economical fashion for topping up the current in both storage rings and still being available >95% of the time for time-resolved short-pulse studies. The Linac-based source is a unique complement to the synchrotron source, providing photons in the same energy range as the synchrotron, but with much shorter (<100 fs) pulses. Specifically, it is envisioned to construct a spontaneous radiation source for hard X-rays, similar to the one that was briefly operational at Stanford (SPPS), whereas for spectroscopy applications a FEL source is planned. These sources ideally complement each other, since the synchrotron is largely used to probe the ground state of matter and the Linac sources serve to uniquely explore the ultra-fast (fs) dynamics and nonlinear processes of matter. Having the Lund Laser Center close by, and a well-established track record of collaborations, is a unique advantage for this field, since there is ample experience with short-pulse lasers and time-resolved spectroscopy.

Scientific applications for the Linac-based sources include fs time-resolved reaction chemistry, photo-biology, phase transitions in solids, magnetization dynamics, combustion and plasma physics, to name a few. Not only are these basic scientific questions, but there is substantial interest expressed by industry concerning technological applications. The chemical industry has expressed great interest in being able to monitor a chemical reaction in real time, whereas for magnetic storage media the ultimate time scale of the magnetic recording may be expanded by orders of magnitude from the current technology. In the VUV range such a source, in combination with a synchronized external laser, will offer unique spectroscopy possibilities for the study of the electron dynamics during a chemical reaction, charge transport and trapping in semiconductors or solar cells, or metal-insulator phase transitions in oxide materials. Dynamic studies of hydrogen bonding are important to improve our understanding of systems ranging from small molecules, such as water, up to large biological complexes. The hard X-ray incoherent source will offer a unique tool for the study of structural dynamics

from phase transitions to melting in condensed matter physics. This source provides substantially larger numbers of photons/pulses than the slicing sources currently operational at the ALS (Berkeley) or SLS (Switzerland). Only the X-FEL at LCLS or DESY can reach higher performance levels.

The Panel also would like to emphasize that the VUV FEL source will provide unique opportunities for single-shot stroboscopic imaging applications in materials and life sciences. The largely coherent FEL source can be used not only in microscopy but also in a holographic (lens-less) imaging setup exploring differing contrast modes, thus allowing images with resolution down to about 10 nm to be obtained, according to the wavelength of the FEL source.

Development of advanced instrumentation for spectroscopy

Traditionally, the groups at Uppsala University have been extremely strong in the development of advanced instrumentation and methods for electron spectroscopy and X-ray emission spectroscopy. These instruments have defined the top standard of performance for this type of instrumentation, leading to very successful commercialization. Photoelectron and soft X-ray photon spectrometers produced by Gammapdata/Scienta in Uppsala have been produced for a world-wide market. The MAX II facility at Lund was an essential ingredient in these developments. MAX IV will have a strong impact on further developments. Several new innovative concepts for both electron and photon spectrometers were presented, which will lead to a substantial advancement of this type of sophisticated instrumentation. These instruments will again push the envelope and set new standards for the performance. It is obvious to add that these advances in instrumentation are intimately related to new scientific achievements. This development is gaining additional momentum by the fact that leading theory groups are located in Sweden, developing new concepts for the interpretation of, for example, resonant inelastic X-ray scattering or core-level photoemission spectroscopy.

Similar conclusions were recently formulated in the previously mentioned evaluation on condensed matter physics in Sweden:

“In many ways the pioneering work in Sweden on the development of instrumentation and methods relevant to surface and interface science follows the long tradition of developments in electron spectroscopy in this country. The achievements are no less for this – their positive impact can now be seen in work performed by many groups world-wide which have assimilated these developments.”

“The very important role that the MAX-lab facilities have had in helping Swedish scientists to play such an important role in the application of synchrotron radiation to surface science also owes much to the work performed by Swedish university groups in developing beamlines and associated end-stations.”

“The effective implementation of specific beamline designs at MAX-lab has done much to bring about world-leading applications of existing techniques as well as new methods.”

GENERAL SCIENTIFIC CONSIDERATIONS

As expressed by the Terms of Reference in Appendix 1, also several questions regarding the general scientific value of a future MAX IV facility were raised. The present section will address these.

The Evaluation Panel is impressed by the content of the “2005 MAX IV Conceptual Design Report” for the proposed project, which gives an excellent overview of the scientific possibilities and needs, as well as the impact of the facility on the scientific community. The MAX IV facility, based on two new electron storage rings, will have an important added value for the current activities in various fields encompassing fundamental and applied research, as well as more industrially related research and machine/detector development. The soft X-ray range will be emphasized by the development of the innovative instrumentation.

With the anticipated performance of the state-of-the-art undulator technology, the choice of building two separate rings of 3.0 GeV and 1.5 GeV is optimal for maximum performance and cost-effectiveness in both hard and soft X-ray regimes. For the IR and VUV applications, the MAX IV will be complemented by the MAX III ring. The cost of moving the MAX III facility is negligible compared to the added scientific value. IR-beamlines may solely be allocated to the MAX III ring. Moreover, the Linac-based source will offer possibilities to study ultra-fast phenomena and non-linear processes.

The availability of a wide spectral range provided by the three-ring configuration will bring scientists from different disciplines together and provide a fertile intellectual environment for interdisciplinary research. The Panel endorses the following areas presented in the CDR and at the meeting: molecular environmental science (MES), biomedical imaging, archaeology, and tomographic microscopy. These are all not only scientifically important but also of strong general interest and high public policy impact.

Every experiment utilising the focussing and high brilliance of MAX IV, such as imaging, nanodiffraction and trace analysis, microdiffraction of biological macromolecules and in material science, will benefit substantially. Examples that can be mentioned involve nanoscience and nanotechnology, catalysis, environmental sciences and topographical imaging. Short exposure times will allow dynamic processes down to the microsecond range to be studied, such as SAXS experiments aimed at protein folding. The Panel supports the proposal of the MAX IV management to look for collaborations on detector development. The MAX-lab has presented a list of focus areas, in Appendix 5, which is supported by the Panel.

In the event that MAX IV will not be built, it is inevitable that the Nordic research community will be negatively affected. The market for excellent professionals for accelerator and beamline science and technology is highly competitive and the most competent staff will migrate to more modern sources. This will have serious consequences for research and education in Sweden and the Nordic countries.

One advantage of combining MAX IV with an FEL facility is that it offers the possibilities to maintain a cutting edge in instrument development. The combination of a synchrotron source jointly with a short-pulse Linac source, which can be expanded into an FEL facility, is unique to the design of the MAX IV project. As mentioned, these sources ideally complement each other, since the synchrotron is largely used to probe the ground state of matter and the Linac sources serve to uniquely explore the ultra-fast (fs) dynamics and nonlinear processes of matter.

COMMENTS ON INFRASTRUCTURE

Frequent and sustained access to a local synchrotron source is an important added value for the Nordic, and possibly Baltic, scientific community. Outstanding science proposals are likely to gain access to other synchrotron labs but not necessarily sufficient beamtime. However, MAX IV will provide a better opportunity for exploratory experiments to be conducted in a timely fashion.

The unique capabilities of the MAX IV storage rings will attract users world-wide. At present, the user community at MAX-lab consists of about 50% Swedish, 25% other Nordic and 25% international users. It is expected that MAX IV will have a similar or more international user community.

With respect to co-localization of MAX IV with a potential ESS neutron facility, the Panel expects a scientifically synergetic complementarity in the areas of materials science, magnetism, soft matter and superconductivity. Both facilities could share the same infrastructure, such as housing, libraries, etc., and therefore facilitate an easy exchange of scientific ideas and concepts. One could also envision joint workshops, educational, and outreach activities. However, neither the need nor the success of MAX IV will depend on having ESS close by.

According to the presentations made at the Panel meeting, we expect a strong and visible involvement of the pharmaceutical/biomedical and chemical industry. Lund and MAX IV are strategically embedded in the southern Scandinavia Medicon Valley area with a large number of pharmaceutical and biotech companies of various sizes. The bigger companies such as Astra Zeneca and Novo-Nordisk Farma have actively contributed to the construction and operation of MAX II and carry out vigorous research programmes. The easy and timely access to a high-performance and local synchrotron facility is of utmost importance to industrial research, and therefore future commitments from industry are highly probable. For example, in addition to pharmaceutical industry, nanoscience and nanotechnology – such as catalysis – is a growing field with a clear industrial interest. It is likely that materials science originating from the oil industry may take advantage and provide regular users. Traditional Nordic industries like forestry and mining remain potential users.

The overall timeliness of the MAX IV project is good. The time schedule presented at the hearing at MAX-lab, Appendix 6, is considered by the Panel to be aggressive but realistic. However, in order to realize the time schedule it is important that the momentum is kept, that the decision on a fu-

ture MAX IV is made rapidly, and that the funding for detailed design and prototyping is made available as soon as possible. The Panel supports the idea that the construction period should overlap the operation of MAX II, in order to maintain access to the facility for the user community. There is clear support from the Lund community and Lund University, where MAX IV already is implemented in the city plan and university strategy.



COMMENTS ON PROPOSED ORGANIZATION AND BUDGET

Regarding the proposed budget for operation of MAX IV, the request for personnel seems low for the number of beamlines and challenging experiments that will be enabled by the state-of-the-art facility. The Panel encourages the management to do a detailed plan to ensure that staffing meets the needs. An average for the modern sources, such as Diamond, is about 5-6 total support staff per beamline. For the machine operation the proposed number seems to be adequate. MAX-lab has excellent staff within both accelerator physics and beamline design and operation.

With the information available, the Panel cannot make any judgement on the proposed organization for construction and operation. However, the track record of constructing and operating earlier MAX facilities is excellent. The management clearly recognizes the challenges associated with the new construction and ongoing operation at MAX II, as well as the significant need for an increase in staff.

As for time-critical points of the MAX IV project, if the strategic decision is made to fund the facility, it is imperative to ensure that the momentum is maintained. In the opinion of the Panel the proposed budget is highly cost-effective, and therefore the proposal should be fully funded as presented.

In case of a serious shortfall of the funds (only 75% funding), it is impossible for this Panel to suggest a cut which would not seriously impair the ability of MAX IV to compete with other European and international synchrotron facilities.



CONCLUSIONS

- The proposed MAX IV facility represents a highly innovative design and will create a first-class facility of world-wide importance. The three optimized rings and a Linac-based source represent a very cost-effective package.
- The user community has an excellent track record in producing high-impact science. The proposed facility will have the potential to attract users world-wide and to build user communities in new scientific areas.
- The scientific programme is strong and effectively coupled to the unique properties of the proposed facility.
- The facility will benefit from the strong pool of industries in the area. There are already well-established ties with industry, and they will be strengthened by construction of the new MAX IV facility.
- The new facility is strongly supported within the university strategy and in the city plan.
- The facility will provide an ideal site for education at technical and advanced scientific levels for the Nordic universities and industry.

The Panel evaluation ends with one single recommendation:

Based on the evaluation of the scientific case presented in the MAX IV Conceptual Design Report and the Lund Hearing, the Panel is unanimous in recommending MAX IV to be funded to the level requested. The funding should commence as soon as possible.

APPENDIX 1

Terms of Reference

Evaluation of the MAX IV proposal

Introduction

The national laboratory MAX-lab in Lund has submitted to the committee for research infrastructure (KFI) at the Swedish Research Council a proposal for the first phase of the scientific programme at a new synchrotron radiation laboratory, MAX IV. The technical concept of the MAX IV laboratory has already been evaluated by a group of specialists appointed by the KFI. The results from this evaluation have been described in a separate report.

The MAX IV proposal constitutes design and construction of two electron storage rings for synchrotron radiation, the relocation of an existing storage ring, a Linac for injection and short-pulse experiments, and the first 15 beamlines and experimental stations. The Linac is also planned to be used for a future VUV/X-ray Free Electron Laser.

The present evaluation is to examine in detail the proposal for MAX IV as presented in the Conceptual Design Report and evaluate its merits. After completion, the results and conclusions of the review will be made public in a written report.

Review Panel

The review will be conducted by a "Review Panel". All members will be internationally recognized experts, with broad views and expertise. None of the members shall be personally and actively engaged in MAX-lab.

The chairperson of the Review Panel is Professor Lars Kloo, KTH. Professor Kloo heads the review and is the rapporteur of the Panel. A research officer from the Swedish Research Council acts as the co-ordinator of the review.

Professor Hans-Åke Gustafsson, Lund University, will take part in the evaluation as an observer representing the KFI. Members of the working group for Molecular, Cellular and Material Research may attend the evaluation as observers. The research councils of the Nordic countries have been invited to send observers to the evaluation.

Review schedule

The review shall be made during the fall of 2006 and the Panel shall have at least one site visit at MAX-lab. A preliminary report shall be presented to the Swedish Research Council not later than November 10, 2006.

Review procedure

The Review Panel shall investigate the general scientific/technical merits of the design for the proposed MAX IV laboratory as well as the proposed budget and time-frame for completing the project. In particular, the strengths and weaknesses of the scientific programme shall be examined and compared to other recently commissioned synchrotron radiation sources. The new areas of science that can be investigated due to the unique qualities of the synchrotron light specified in the MAX IV design should clearly be identified. Any scientific, technical, organizational, and economic risks or shortcomings of the project should be pointed out. The figures of merit of the MAX IV laboratory and the cost-effectiveness shall be compared to other recently funded and planned synchrotron radiation laboratories.

The Review Panel is asked to write a report of its opinion about the MAX IV proposal. In this report the Panel is requested to:

(Scientific issues)

- Evaluate, from an international point of view, the scientific value of the proposed project for physics, chemistry, biology, engineering and other relevant disciplines.
- Comment on the role the laboratory may have for development of interdisciplinary research.
- Evaluate the scientific justification of the proposed project in the context of international scientific programmes of existing and planned laboratories with similar aims of research.
- In particular the review panel is asked to make a statement about the choice of electron energies for the two new storage rings in view of the proposed scientific programme and the fact that MAX III will be transferred to the new site.
- Give a statement about the experiments that will benefit most from the high brilliance of the storage rings and in particular identify experiments that may reach unique performance.
- Comment on the consequences for the Swedish/Nordic research community if MAX-lab is not upgraded with the proposed MAX IV facility.

- Comment on the possible advantages of combining a synchrotron radiation laboratory with a future FEL facility.
- Comment on whether any important scientific developments and applications within synchrotron radiation research are missing in the proposal.

(Infrastructure issues)

- Evaluate, as an alternative to the construction of MAX IV, the possibility for Swedish and Nordic scientists to obtain sufficient beamtime at existing and planned synchrotron radiation sources by scientific, technological and economic involvement in the construction of beamlines at those facilities.
- Estimate the potential for the MAX IV laboratory to attract international users and partners.
- Comment on the potential benefits of having a synchrotron radiation source of the MAX IV kind in Sweden, including the impact on the industrial and public sector.
- Comment on the advantage/disadvantage of the opportunity that the MAX IV facility may be located in the same area as the European Spallation Source.
- Comment on the parts of the proposed research programme that may attract industrial users and if so also indicate the industrial sector. The panel is asked to investigate the possibility for small and medium size companies to use the laboratory. For larger industrial users, which already successfully are using synchrotron radiation, the panel is asked to comment on the new research possibilities that MAX IV may give.
- Evaluate the appropriateness of the time schedule for the proposal.

(Financial and organizational issues)

- Evaluate the estimated running costs of the facility.
- Evaluate the demands for personnel, equipment, and operating costs at the proposed laboratory.
- Give an estimate for the manpower, indicating critical competences, needed to run MAX IV including beamlines and experimental stations.
- Comment on the timeliness of the proposal and the suggested time schedule for construction.
- Assess the proposed organization for construction and operation of the facility.
- Identify critical points during the MAX IV project that prospective funding agencies need to be aware of.

- The panel is also asked to suggest priorities of the project based on an estimate that only 75% of the requested funding for can be obtained. The cost-reducing suggestions may for example be related to the number and priorities of beamlines, focus on particular scientific areas, changing the number of electron storage rings or any other suggestion the Panel finds appropriate.

APPENDIX 2

Short CV's for the experts

Prof. Maria Arménia Carrondo

- Full Professor at Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa. Current address: ITQB – Av. da República, 2784-505 Oeiras, Portugal
 - Born in V. N. De Famalicão, Portugal, in 1948
 - Chem. Eng. by University of Porto, Portugal; Ph.D. in Chemical Crystallography, Imperial College of Science and Technology, University of London, UK
-

Special assignments

Full Professor at Instituto de Tecnologia Química e Biológica (ITQB), Universidade Nova de Lisboa (1998-present); Associate Professor at Instituto Superior Técnico (IST), Universidade Técnica de Lisboa (1979-1998).

Leader of the Macromolecular Crystallography Laboratory at ITQB (1988-present), Elected EMBO member in 2000; European Medal for Bio-Inorganic Chemistry in 2004. Vice-Director of ITQB (1996-2005). Member of the Executive Direction of IST (1984-1987).

Representative of the Portuguese Government at the ESRF Council (1998-2002). Representative of the Minister for Science and Technology in the process that led to the Portuguese membership of ESRF in 1997. Users representative at the EC Round-Table for synchrotrons (1991-1996).

Member of the ESRF Review Committee in Life Sciences - Protein Crystallography (2000-2003). Member of the Review Panel of the EMBL Hamburg Outstation in 2003. Member of the Priorities Committee of the EMBL Hamburg Outstation since 2005.

Editor of *Journal of Biological Inorganic Chemistry* since December 2001.

Officer of the Executive Committee of the International Union of Crystallography (1999-2005) and Chair of the IUCr Sub-Commission on the Union calendar (2002-2005). Officer of the Executive Committee of the European Crystallography Association (ECA) (1997-2000).

Member of the Organizing and Programme Committees of the Eurobic8, Aveiro, Portugal, 2006. Organizer of the EU courses BioCrys on “Fundamentals of modern methods in Biocrystallography”, Oeiras, 2002, 2004 and 2006. Vice-President of the Organizing Committee of the FEBS meeting, Lisbon, 2001. Chair of the Organizing Committee of ECM 17, Lisbon, 1997. Member of the Programme Committee of ECM 16, 1995, Lund and member of the Advisory Board for ECM 18, 1998, Prague, Czech Republic and Member of the Programme Committee for ECM 19, 2000, Nancy, France. Founding Member of the Special Interest Group within ECA on Macromolecular Crystallography and Secretary between 1998 and 2001. Chair of this SIG since 2006. Vice-President of the Portuguese Biochemical Society (1998-2004).

Representing ITQB as partner on the EU integrated project SPINE2-Complexes, on the EU Infrastructure Cooperation Network, MAX-INF2 and associated TID centre to the EU integrated project BIOXHIT.

Special Scientific Interests

Protein Crystallography. Structural studies of electron transfer proteins, metalloproteins and metalloenzymes and proteins with pharmacological and biomedical applications. Application of methods involving data obtained in synchrotrons, namely MAD, SAD and *ab initio* methods.

Prof. Yvan Bruynseraede

- Professor Emeritus of Physics, Past Chairman Laboratory of Solid-State Physics and Magnetism, Department of Physics and Astronomy, Catholic University of Leuven (KULeuven), B-3001, Heverlee, Belgium
 - Born in Oostende, Belgium, in 1938
 - MSc and PhD in Physics, KULeuven, Belgium
-

Special Assignments

Postdoctoral and Associate Fellow, CERN, Geneva, Switzerland (1969-1972); Lecturer and Professor of Physics, KULeuven, Belgium (1972-2003); Chairman, Laboratory of Solid-State Physics and Magnetism, KULeuven (1993-2003); Chairman, Research Council, KULeuven (1990-1995); Fellow, American Physical Society (1990-present); Member, Editorial Board, Physical Review Condensed Matter Physics (1991-1997); Member, Council Research Management, KULeuven (1995-2006); Chairman, Expert Research Committee, Flemish Interuniversity Council VLIR (2000-2003).

Member (1988-present) and President (1999-2000) of the Royal Flemish Academy of Belgium for Science and the Arts; Member, Council ESRF Grenoble, France (1988-1998); Chairman, Belgian Physical Society (1989-1991); Member, Board Belgian Nuclear Research Centre SCK.CEN Mol (1991-present); Member, Board European Physical Society EPS, France (1997-2001); Member, Board Institute for Radioactive Elements IRE, Belgium (1999-2005); Member, European Academy of Sciences and Arts Vienna, Austria (2001-present); Member, Board of Regents KULeuven (2003-present); Member, The Royal Society of Arts and Sciences in Gothenburg, Sweden (2005-present).

Member, Committee of Solid State Physics, National Fund for Scientific Research NFWO, Belgium (1984-1994); Member, Committee National & International Relations, Flemish Council for Science Policy VRWB (1990-1994); Member, Committee Science Management VRWB (1994-present); Chairman, Scientific Advisory Committee SCK.CEN Mol (1997-present); Member, International Advisory Committee IFIMUP, Porto, Portugal (1998-present); Member, Expert Advisory Committees of the VR and SSF, Stockholm, Sweden (2000-present); Member, International Reviewing Committee Grenoble High Magnetic Field Laboratory GHMFL, France (2002); Member, Expert Advisory Group EU-FP6-NMP, Brussels, Belgium (2002-2006); Member, Strategic Advisory Committee, Flemish Institute for Technological Research VITO, Mol, Belgium (2002-present); Member, ESF Review Panel Fundamentals of NanoElectronic (FoNE), Strasbourg, France 2005; Chairman, ESF Review Panel Self-Organised NanoStructure (SONS), Strasbourg, France (2005); Member International Review Committee Physics Research at RUNijmegen/TUEindhoven, The Netherlands (2005); Member, International High-Level Science Panel Linnaeus Grants of the Swedish VR, Stockholm, Sweden (2006); Member, DoE Panel Basic Research Needs for Superconductivity, Washington, USA (2006).

Specific scientific interests

Electrical, magnetic and optical properties of mesoscopic and nanoscopic structures at very low temperatures and very high pulsed magnetic fields; superconducting vortices in thin films; superconducting/magnetic heterostructures; magnetic interactions in thin films, nanostructures, superlattices and clusters; characterization of magnetic structures with X-ray diffraction; scanning probe microscopy studies of surfaces and interfaces.

Prof. Dr. Dr. h.c. Wolfgang Eberhardt

- Born July 27, 1950 in Lieser, Germany
 - Scientific Director of BESSY m.b.H
 - Full Professor in Experimental Physics at the Technical University Berlin
 - 1978, Ph.D. in physics, Universität Hamburg
 - 2003 Honorary PhD, Uppsala University (Sweden)
-

Special Assignments

Teaching Assistant in theoretical physics, Justus Liebig Univ., Giessen (1972-1974).

Diplom Physiker, II. Inst. für Exp. Physik, Universität Hamburg (1974-1978).

Research Investigator and Assistant Professor of Physics (1980), University of Pennsylvania, Philadelphia, USA (1978-1981), Associate Physicist, Physics Dep., Brookhaven National Laboratory (1981-1982), Staff Physicist and Senior Staff Physicist (1986), Exxon Research and Eng. Co., Annandale NJ 08801, USA (1983-1990).

Director, Institute "Electronic Properties" at the IFF, KFA-Jülich and Professor of Physics, University of Cologne, Germany (1990-2001); Scientific Director, BESSY mbH Berlin, Germany and Professor of Physics, Technical University of Berlin, Germany (2001-present).

Guest Scientist, Physics Dept., Brookhaven National Laboratory (summer 1983), Guest Scientist, BESSY, Berlin (summer 1987), NSLS Users executive committee (elected member), NSLS Brookhaven (1983 to 1988), ALS Users executive committee (appointed member), ALS Berkeley (1987 to 1990), BESSY Beirat Grundlagenforschung, member, 1990-1994, Chairman (elected) Gordon Research Conference on Electron Spectroscopy (1992), DAAD HSPII Selection-Committee (1992-2001), Member of various NSF, DOE, DFG, and BMBF review panels, National Committee for Research with Synchrotron Radiation, member (1993-present), Co-Editor, Applied Physics A, Springer Verlag (since 1994), BESSY, Board of Supervisors (1995-1999), HASYLAB, Advisory committee Synchrotron Radiation (1995 until 1997, chair 1996 and 1997), Science Advisory Committee of the MPI for Solid State Research, Stuttgart (1995-2004), ESRF, Science Advisory Council (1996-1999), Peter Wall Institute, UBC Vancouver, Scientific Council (1996-1999), ESRF, Beamtime Review Committee (Electronic Structure and Magnetism) (1998-2000), ALS Berkeley, Science Advisory Committee (1998-present), PSI-Swiss Light Source, Science Advisory Council (2001-present), SSRL (Stanford), Science Advisory Committee (2005-present).

Specific scientific interests

Electronic structure of atoms, molecules, and solids determined by photoemission and synchrotron radiation related techniques; Development of angle resolved photoemission to study the band structure of solids, surfaces and interfaces; Electronic structure and magnetism of thin films and nanostructures; Fs-magnetization dynamics; Electronic properties and structure of clusters; Core electron excitation and dynamic screening processes in molecules and solids; Fs-2-photon-photoemission spectroscopy of clusters and solids; Scattering and holography with coherent synchrotron radiation.

Dr. Michael Grunze

- Professor for Applied Physical Chemistry and Director at the Institute of Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany
 - Born in Mühlheim/Ruhr, Germany, in 1947
 - Ph.D. and Habilitation at Freie Universität, Berlin, Germany
-

Special Assignments

Postdoctoral Research Fellow, University of Munich, Germany, and Queen Mary College, University of London, United Kingdom (1975-1976); Group Leader and Scientist, Fritz-Haber-Institut, Max-Planck-Gesellschaft, Berlin, Germany (1978-1984); Visiting Scientist, IBM Research Laboratories, San Jose, California, USA (1981); Visiting Professor of Physics, University of Osnabrück, Germany (1982); Director, Laboratory for Surface Science and Technology (LASST), University of Maine, USA (1985-1987); Adjunct Professor of Chemistry, Department of Chemistry, University of Maine, USA (1984-1988); Professor of Physics, Department of Physics, University of Maine, USA (1984-1988); Professor, Lehrstuhl für Angewandte Physikalische Chemie, University of Heidelberg, Germany (1987-present); Director of the Institute of Physical Chemistry, University of Heidelberg, Germany (1987-present); Visiting Professor, Department of Biological Chemistry, Harvard University, Cambridge, USA (1996); Adjunct Scientific Staff, The Jackson Laboratory, Bar Harbor, Maine, USA (2001-present); Chairman, Biomaterial Interface Division, AVS Science and Technology Society, USA (2002-2003); Chairman, Scientific Advisory Council Synchrotron Radiation Source BESSY, and Member of the Scientific Advisory Council Hahn-Meitner-Institute, both Berlin, Germany (2002-2004); Co-Director, Institute for Molecular Biophysics, University of Maine, USA (2003-2006); Adjunct Professor

of Physics & Member of the Graduate School, University of Maine, USA (2003-present), Member of the ESRF Scientific Advisory Council, Grenoble, France (2006-...).

Fulbright Fellowship (1968-1977); Liebig-Habilitations-Stipendium (1975-1977); Otto-Klung-Prize for Outstanding Contributions in Physical Chemistry (1976); Guptill Memorial Lecture, Dalhousie University, Halifax, Canada (1997); JG McGregor Distinguished Scientist, Dalhousie University, Halifax, Canada (1999); College De France Invited Lecturer, Paris, France (2001); Max-Planck-Research-Award (2003); Fellow of the American Vacuum Society (2005); ISIS Distinguished Lecturer, University of California, USA (2006).

Special Scientific Interests

Surface chemistry and interface physics; biocompatible and antifouling surface coatings; adhesion science; self-assembly of organic mono- and multilayers; non-linear optical laser spectroscopy on surfaces; photoemission; X-ray absorption and X-ray emission spectroscopy; X-ray microscopy; in-line holography; biochemical sensors.

Present Research Interests: Experimental studies and simulations of organic films; polymer adhesion; synthesis of novel functional molecules for surface modification; biomaterials; X-ray absorption spectroscopy and microscopy and X-ray emission spectroscopy using synchrotron radiation; neutron scattering; theory of self-assembling films; non-linear optical laser spectroscopy on surfaces (SHG and SFG); protein and cell interactions with artificial surfaces; protein adsorption kinetics; protein resistant and “inert” surfaces; cell adhesion; acoustic and optical biosensors; theory of biomolecule/surface interactions; X-ray microanalysis of biological tissue; biophysical aspects of glaucoma; chemical nanostructures; environmental effects of nanoparticles, marine antifouling coatings.

Prof. Britt Hedman

- Professor and Deputy Director, Stanford Synchrotron Radiation Laboratory, Stanford University, 2575 Sand Hill Road, Menlo Park, CA 94025, USA
 - Born in Skellefteå, Sweden, in 1949
 - M.Sc. and Ph.D. in Chemistry, Umeå University, Sweden
-

Special Assignments

Research Associate and Lecturer, Department of Chemistry, University of Umeå, Sweden, 1978-1982; Faculty Research Associate (Asst. Professor equiv.), Department of Chemistry, University of Umeå, Sweden, 1982-1985; Senior Research Associate, Stanford Synchrotron Radiation Laboratory, Stanford University, 1985-2001; Adjunct Professor of Bioinorganic Chemistry, Department of Chemistry, University of Umeå, Sweden, 1996-2002; Assistant Director, Stanford Synchrotron Radiation Laboratory, Stanford University, 2001-2005; Professor, Stanford Synchrotron Radiation Laboratory, Stanford University, 2002-current; Deputy Director, Stanford Synchrotron Radiation Laboratory, Stanford University, 2005-current.

Member of the Research Educational Board at the Institute of Chemistry, University of Umeå, Sweden, 1976-1978; Member of the Board for the Institute of Chemistry, University of Umeå, Sweden, 1978-1980; Member of the Swedish Chemical Society, 1971-1983; Member of the American Crystallographic Association, 1982-current; Member of the American Chemical Society, 1985-current; Member of the International Committee on Standards and Criteria in X-ray Absorption Spectroscopy 1988-1994; Member of the International Union of Crystallography *Ad interim* Commission on Synchrotron Radiation, 1990; Member of the International Union of Crystallography Commission on Synchrotron Radiation, 1990-1996; Expert Advisor, Appointment Board, Faculty of Agricultural Science, Swedish University of Agricultural Science at Uppsala, Sweden, Lecturer Appointment in Chemistry, June 1996; Member of the International Union of Crystallography Commission on XAFS, 1996-1999; Expert Advisor, Appointment Board, Faculty of Science, Lund University, Sweden Professorship in Synchrotron Radiation Instrumentation, 1998; Member of the Environmental Molecular Sciences Laboratory Advisory Committee, Pacific Northwest National Laboratory, 1998; Member, International XAFS Society, Executive Committee, 2000-2006; Member, Committee on Research, Stanford University, 2000-2001; Member, BioCAT NIH NCRR Advisory Committee, Advanced Photon Source, Argonne National Laboratory, 2001-current; Member, NIH NCRR Special Study Section Site Visit Team for NCRR Research Resource, 2002; Member, International Scientific Program Committee, IUCr2005, XX Congress of the International Union of Crystallography, Florence, Italy, 2005; Member, Scientific Advisory Committee, Canadian Light Source, Canada, March 2005-current; Co-chairperson, XAFS13, 13th International Conference on X-ray Absorption Fine Structure, Stanford University, 2006.

Specific scientific interests

Development and applications of synchrotron radiation-based X-ray ab-

sorption spectroscopy, with scientific emphasis on the study of the electronic and structural aspects of metal ion active sites in bioinorganic and biological systems, with the goal to understand biological function.

Dr. Chi-Chang Kao

- Chairman, National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (BNL), Upton, New York, 11973, USA
 - Adjunct Professor, Physics Department, Stony Brook University
 - Born in Taipei, Taiwan, in 1958
 - Ph.D. in Chemical Engineering, Cornell University, USA
-

Special Assignments

Interim Chairman, NSLS (2006); Deputy Chairman, NSLS (2005-2006); Associate Chairman for User Science, NSLS (2001-2005); Senior Physicist, BNL (2001-); Physicist with tenure, BNL (1997-); Physicist, BNL (1994-1997); Associate Physicist, BNL (1992-1994); Assistant Physicist, BNL (1990-1992); Postdoctoral Research Associate, BNL (1988-1990).

Member, Steering Committee, Taiwan Photon Source (2006); Member, Scientific Advisory Committee, Stanford Synchrotron Radiation Laboratory (2005-); Member, Advisory Committee of Carnegie-DOE Alliance Center (CDAC) (2004-); Member, the College of Reviewers for the Canadian Research Chairs program (2003-); Member, Advisory Committee of COMPRES – “the Consortium of Materials Properties Research in Earth Science”(2002-); Advisor, Taiwan Synchrotron Radiation Research Center /SPring-8 project (1999-).

Member, International Advisory Committee. The 6th International Conference on Inelastic X-ray Scattering (IXS2007), May 7-11, 2007, Awaji, Japan; Member, International Advisory Committee, The 9th International Conference on Surface X-ray and Neutron Scattering (9SXNS), July 16-20, Taipei, Taiwan; Member, International Advisory Committee, The 13th International Conference on X-ray Absorption Fine Structure (XAFS13), July 9-14, Stanford, CA; Member, Technical Program Committee, The Ninth International Conference on Synchrotron Radiation Instrumentation (SRI2006) Meeting, May 28-June 3, 2006, Daegu, Korea.

Special Scientific Interests

Development of new experimental techniques using synchrotron radiation, and their applications to condensed matter physics and material sciences,

in particular, soft X-ray resonant magnetic scattering for magnetism and magnetic material research, and high-resolution inelastic X-ray scattering for electronic structures of condensed matter under extreme conditions.

APPENDIX 3

Agenda for the MAX IV Hearing in Lund, October 19-20, 2006

(Wednesday, October 18)

Approx 19.30

Dinner at the hotel or a nearby restaurant.

Thursday, October 19, at MAX-lab

8.40

Taxi to MAX-lab

9.00 – 10.30

Introduction

10.30 – 11.00

Closed session, Coffee

11.00 – 12.30

Scientific motivation and beamline descriptions:

- Materials Science
- Life Sciences
- Industrial research

12.30 – 14.00

Closed session, Lunch

14.00 – 15.30

Scientific motivation and beamline descriptions, contd.:

- Fundamental processes – Dynamics – Time-dependent phenomena
- Solids, surfaces and interfaces
- Nanoscience

15.30 – 16.00

Closed session, Coffee

16.00 – 17.00

Scientific motivation and beamline descriptions, contd.:

- Interdisciplinary research
- Novel X-ray spectroscopic tools

17.00 – 18.00

Infrastructure aspects

18.30 – 19.30

Dinner at the hotel

19.30 –

Work with the report (at the hotel)

Friday, October 20, at MAX-lab

8.40

Taxi to MAX-lab

9.00 – 12.30

Work with the report. (MAX-lab staff available for questions)

12.30 – 13.30

Lunch

13.30 – 16.00

Work with the report. (MAX-lab staff available for questions)

APPENDIX 4

Proposed MAX IV budget

MAX IV: Cost estimates (October 2006)

This document summarizes the estimated investment and operational costs for the MAX IV facility. The present estimates do not include costs that are specifically related to the Free Electron Laser project.

The cost of the building is included in two ways. For completeness an estimate of the investment cost is provided in connection with the investment budget. However, we foresee that the cost of the building will be paid in terms of a rent to the provider of the building. The total rent is included in the estimated operational budget. This implies that also the capital cost of the building is covered by the operational budget.

Investments

The accelerator costs cover the new 1.5 GeV and 3.0 GeV rings, the 3.0 GeV Linac injector and the relocation of the MAX III 0.7 GeV ring.

The beamline costs are based on 13 new beamlines and a set of relocated beamlines. The present cost estimate is based on six relocated MAX II beamlines. The relocation of MAX III will involve three or four beamlines.

Costs related to the use of the present MAX-lab personnel are not included. All other personnel costs during the build-up period are contained in the investment budget.

		kSEK
Accelerators	3 GeV Ring	140000
	1.5 GeV Ring	120000
	0.7 GeV Ring	5000
	3 GeV Linac	153000
	Project services	150000
	Sum	568000
	Contingency 25%	142000
	Total	710000

		kSEK
Beamlines	Beamline costs	516560
	Project services	100000
	Sum	616560
	Contingency 15%	92484
	Total	709044
Additional facilities	Laboratories	100000
	Offices	5000
	Common facilities	10000
	Project services	50000
	Sum	165000
	Contingency 15%	24750
	Total	189750
Total MAX IV		1608794
Buildings		625000
Total including buildings		2233794

MAX IV: Operational costs

The estimated operational cost is based on the assumption that MAX IV will operate within the administrative framework of Lund University. It is also assumed that the payment of the rent and the management of the general facilities are handled by Lund University. The estimates contain costs for administrative and other support functions at the same relative level as for the present operation. A university overhead at the present level (6%) is foreseen.

Of the 175 staff included in the present budget, 54 are accelerator staff, 65 are staff linked to specific beamlines and 25 are staff for general beamline support. The remaining staff is involved in management, administration, safety, construction and other general support functions.

		kSEK
Salaries		97515
General services		10600
Machine and beamline operation		37000
Overhead		9263
Operation excluding rent		154378
Rent including electricity		84862
Total		239240

APPENDIX 5

Suggested focus areas of the MAX IV facility

The proposed MAX IV synchrotron radiation facility is a combination of three storage rings and a 3 GeV Linac. The three rings will operate at 0.7, 1.5 and 3 GeV respectively. This will give the opportunity to characterize, in one facility, all aspects of materials covering both electronic and atomic structure. The unique feature of this complex is that it has unprecedented brilliance achieved by a small electron beam giving excellent **focusing and coherence** properties. In addition the brilliance will give very high photon fluxes allowing time-resolution from **picoseconds and upwards**.

The above-mentioned properties will lead to new opportunities for leading-edge research in imaging and nanofocussed probing, including tomographic mapping with chemical specificity.

1. The nanotechnology field is rapidly developing, driven by the need for energy saving and environmental measures. Nanofocussing will be achieved both at the diffraction-limited 1.5 GeV ring and at the 3 GeV ring. The design will allow focusing to 10 nm and beyond for energies up to ~ 40 keV. This will allow experiments with **nanowires, nanocarbon materials, nanophotonics, nucleation** studies as well as studies **in-situ of crack propagation and interactions at surfaces and grain boundaries**. This will be an essential component in the design of new functional materials and allow formulating models for new processing of materials. Mapping with chemical speciation of single cells or waste products will allow detection limits from now in the ppm range down to ~ 100 ppb (parts per billion). The design allows convenient choice of focusing conditions.
2. The pharmaceutical industry and biosciences strongly depend on the structure determination of macromolecules and their folding and rearrangement kinetics. In this area the extreme flux and collimation will allow rapid data collections of **hundreds of compounds per day** and the proposal recognizes the need for automated procedures in this field. Studies of both crystals and solutions are important, and thus **crystallographic and small-angle scattering** techniques will benefit from the superior collimation.
3. The flux and focussing will also contribute to the studies of materials under non-ambient conditions. **High-pressure studies and studies in reac-**

tion cells are of growing importance and the facility will here advance the possibilities.

4. In the field of ultra-fast science the Linac-based beamline will be the most brilliant fs X-ray source in Europe in 2010. It will also provide a unique fs broadband X-ray source.
5. The soft X-ray community has an excellent track record. There are for instance ideas of a sub-meV X-ray scattering beamline at the 1.5 GeV ring. There may also be opportunities of holographic mappings using a beam-splitter instead of a pinhole.

The above points highlight some of the new opportunities created by the new facility. However, it should be recognized that many experiments needing synchrotron radiation may not be of fundamental breakthrough character in terms of new scientific novelty but of essential importance for further scientific and technological development. New areas of science using synchrotron radiation are emerging particularly in, for instance, environmental science and areas of cultural heritage. This will further increase the need for capacity. The need for a local source of unique capability and efficiency is thus paramount for development. MAX IV will be a Nordic focal point for interdisciplinary research and research education in natural sciences. A continued and further strengthened synergy with the European high-energy rings is foreseen.

APPENDIX 6

Proposed beamlines and time schedule of construction

Tentative list of priority for the MAX IV beamlines (total costs MSEK):

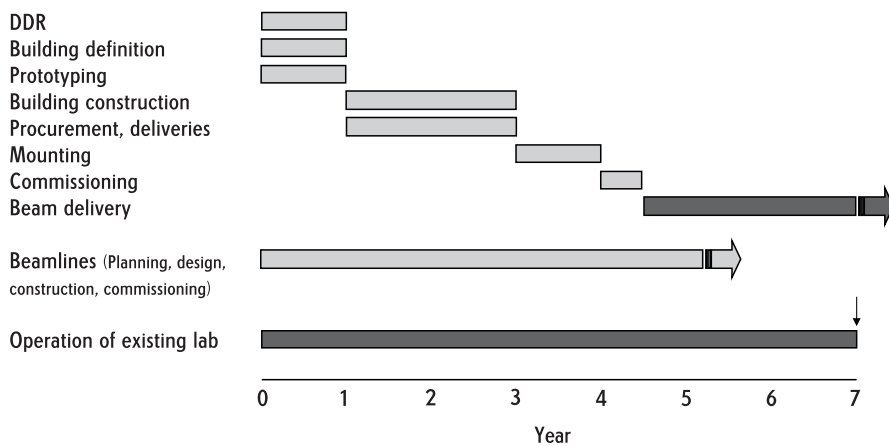
- 1 Nano-2: Diffraction, Imaging and μ -tomography
- 2 MX-2: Macromolecular Cryst.: Microfocus
- 3 High-resolution Powder Diffraction and SAXS/WAXS
- 4 Ultra-high-resolution VUV Scattering (1.5 GeV)
- 5 SPPS (3 GeV Linac)
- 6 Nano-1: Microscopy and Spectroscopy
- 7 Microspot spectroscopy
- 8 MX-1: Macromolecular cryst.: High-throughput and phasing
- 9 Very-high-resolution soft X-ray Spectroscopy
- 10 Soft X-ray Microscopy (1.5 GeV ring)
- 11 Materials Science (wiggler)
- 12 Soft X-ray Gas Phase Spectroscopy (1.5 GeV ring)
- 13 Magnetism
- 14 Soft X-ray Spectroscopy and Surface Reactions (1.5 GeV)
- 15 Relocation of MAX II Beamlines
- 16 Relocation of MAX III Beamlines

The design choice of two rings on top of each other is based on three main considerations.

- 1 The need to access a complete energy range in the most optimal way.
- 2 The substantial savings in building costs with improved performance.
- 3 The synergy effect of common laboratory and infrastructure in close proximity.

For a complete characterization of materials as regards both their electronic and atomic structures the wide energy range is needed while also ensuring that the complementary studies are performed close in time and preferably on identical samples. Combination studies are anticipated in succession. However, simultaneous studies in the different energy ranges need further feasibility investigation.

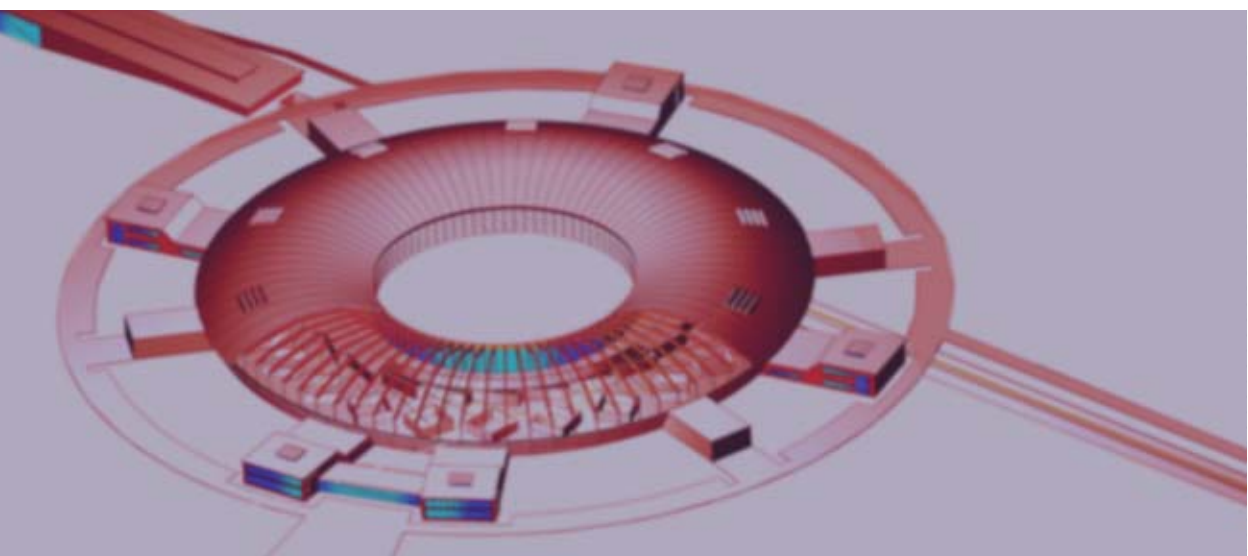
Time plan



Synchrotron-based research has moved from being a challenge within accelerator physics alone to becoming a versatile and widespread scientific tool. Today, a state-of-the-art light source attracts a broad range of scientific communities with the unique experiments that can be performed at synchrotron radiation sources.

The MAX-laboratory in Lund has proposed a new 4th generation synchrotron radiation facility named MAX IV. MAX IV, through its high brilliance, will allow experiments probing structural and physical phenomena at nanometer scale spatially and the evolution of fast dynamic processes at femtosecond scale temporally. Thus, fundamental insights will be obtained to the benefit of a wide range of scientific disciplines.

A panel of international experts has reviewed the scientific case for a MAX IV facility and the result of their evaluation is presented in this report.



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