Somewhat

UTILIZING THE ULTRA-LOW EMITTANCE FIRST PHASE BEAMLINES AT MAX IV

Y. Cerenius
MAX-laboratory, Lund University, Sweden

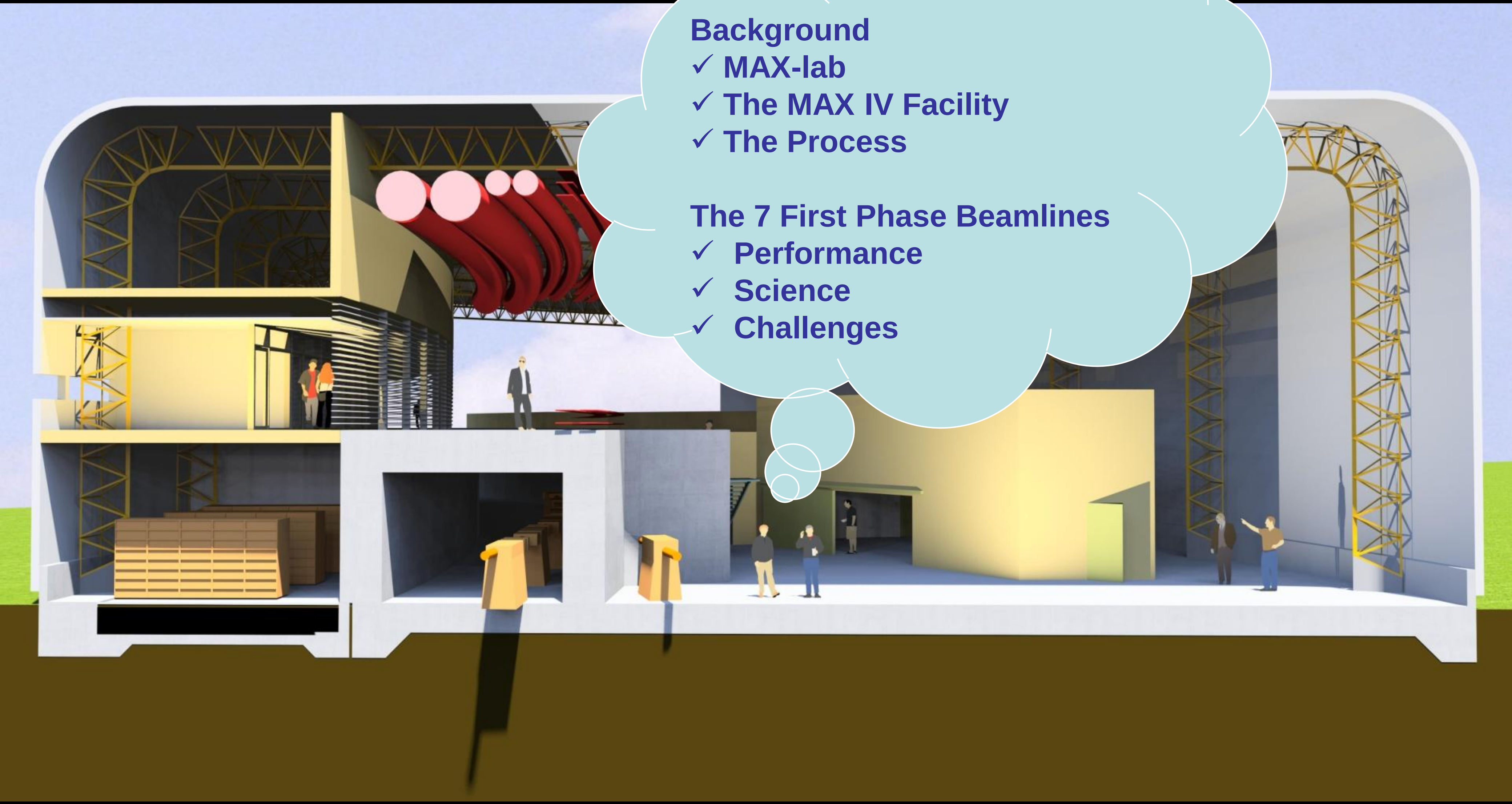
The ground breaking ceremony for the next Swedish synchrotron light source, the MAX IV, took place the 22nd of November last year. When the MAX IV facility will be in operation it will be succeeding the present MAX I, II & III storage rings and consist of two state-of-the-art storage rings, one larger (528 m in circumference) operating at an energy of 3 GeV and one smaller (96 m in circumference) 1.5 GeV ring optimized primarily for lower photon energies. The first user activity is, however, expected to take place on the Short Pulse Facility (SPF) which is situated on the extension of the linear accelerator (linac). The linac will thus be providing both storage rings with electrons in topping up mode as well as it will serve as an electron source for the SPF. There, the electron bunches from the linac will be utilized to produce short (femtoseconds) spontaneous X-ray pulses. This facility could be in operation at a very early stage of the project. Later, there is the option that the linac could be used as a source for a Free Electron Laser (FEL) in the UV and X-ray spectral range. Fully equipped, the new facility will be accommodating about 30 beamlines for research in a wide range of disciplines. The main radiation source of MAX IV, the 3 GeV ring[1], will be an ultra-low emittance (0.24 nmrad) ring for the generation of high brilliance soft- and hard X-rays. The storage ring is designed to meet the requirements of state-of-the-art insertion devices which will be installed on the 19 available 5 m long dispersion-free straight sections. On the 3 GeV ring these insertion devices will deliver an outstanding brilliance (up to 10^{21} photons/(s mrad^{2}mm^{2}0.1%BW)) in an energy range of ~ 200 eV to 30 keV while lower energies will be covered on the 1.5 GeV storage ring. The unique properties of the storage ring creates a number of different opportunities for the MAX IV beamlines, such as focusing down to extremely small beam sizes, combining a small beam size with a low divergence or going for an extreme resolving power while keeping a high photon flux on a small spot. The MAX IV beam will also have a very high degree of coherence. At present (March 2011) there is an ongoing prioritization and funding process for the first phase beamlines. During this process, a set of 10 high profile proposals have been selected and evaluated in several steps, showcasing in different aspects the full potential of the new facility. Out of these 10 it is expected that 6 or 7 of will be selected in the near future. Obviously, these can only be considered to be a subset of the portfolio of the required beamlines for the mature MAX IV project and many important experimental techniques are missing.

At the XLVI Zakopane School of Physics there will be a brief overview of the MAX facility. The selected first phase beamlines and their unique properties, exploring the ultra-low emittance of the MAX IV facility will be presented to some detail.

[1] S. C. Leemann, Å. Andersson, M. Eriksson, L.-J. Lindgren, E. Wallen, J. Bengtsson, A. Streun, Beam dynamics and expected performance of Sweden's new storage-ring light source: MAX IV, Phys. Rev. ST Accel. Beams (2009) 12 [12] 1200171:1-15

[2] Detailed Design Report on the MAX IV Facility,:
http://www.maxlab.lu.se/local/maxiv_ddr/MXAIV_DDR_Master_Subs/DDR_pdf_documents_100406.html

First Phase Beamlines at MAX IV



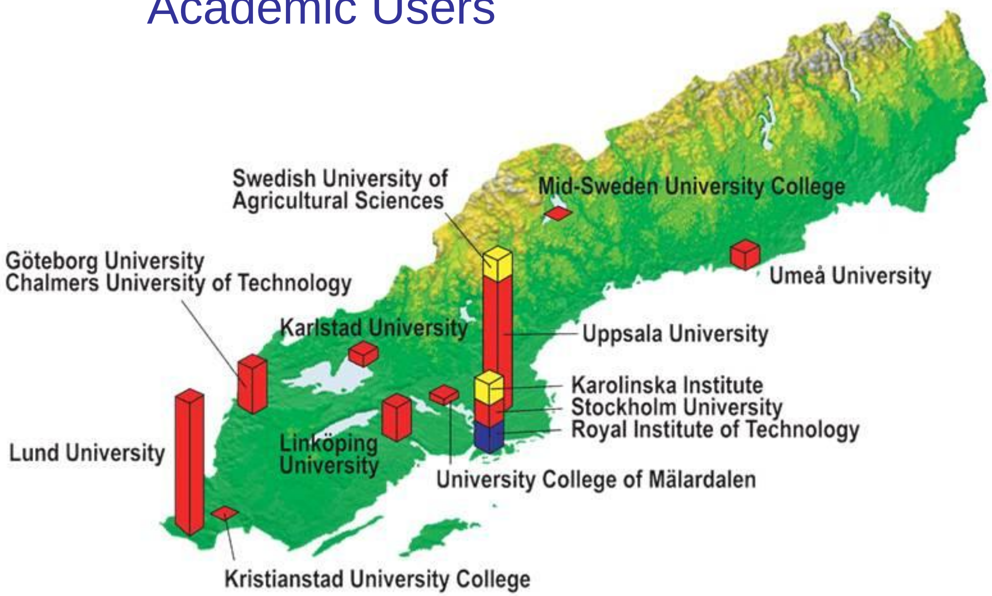
Background
- ✓ MAX-lab
- ✓ The MAX IV Facility
- ✓ The Process

The 7 First Phase Beamlines
- ✓ Performance
- ✓ Science
- ✓ Challenges

MAX-lab, One Out of Two Swedish National Laboratories

- Operated by: Swedish Research Council (VR) & LU
- National Laboratory –> ”open access”

Academic Users



& Commercial Users

Tetra Pak PROTECTS WHAT'S GOOD™
AkzoNobel Tomorrow's Answers Today
BONE SUPPORT
HALDOR TOPSØE
SARomics
Colloidal Resource
novo nordisk®
AstraZeneca

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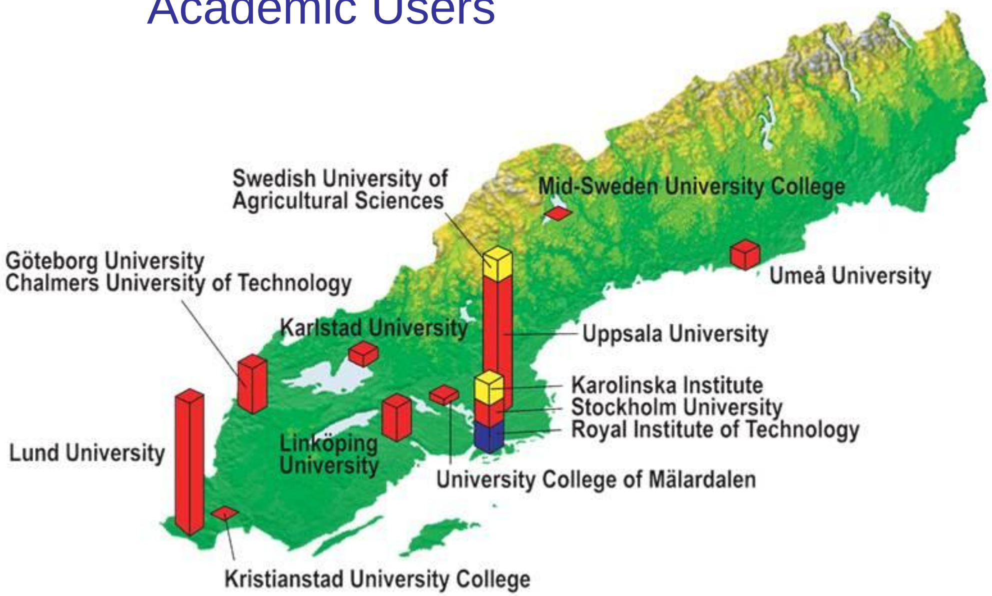
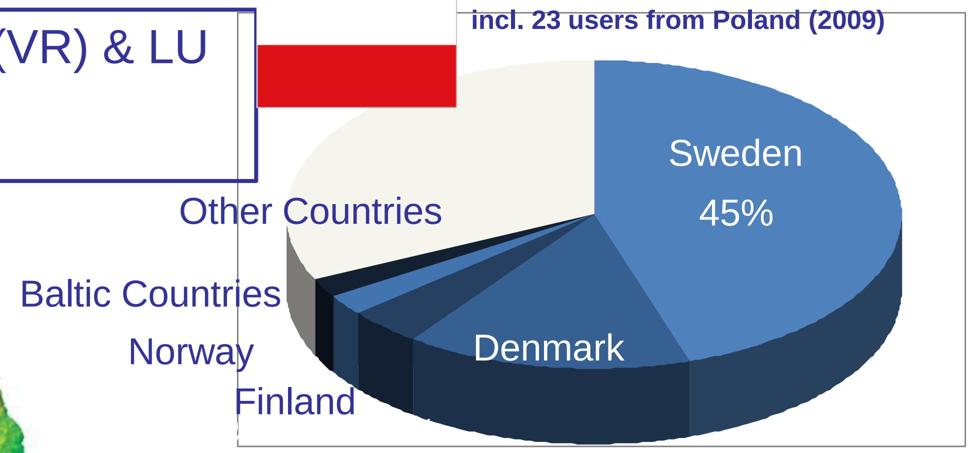
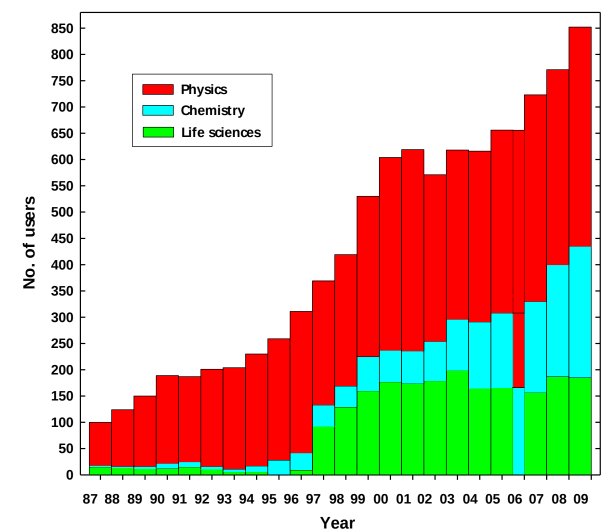
Academic Users

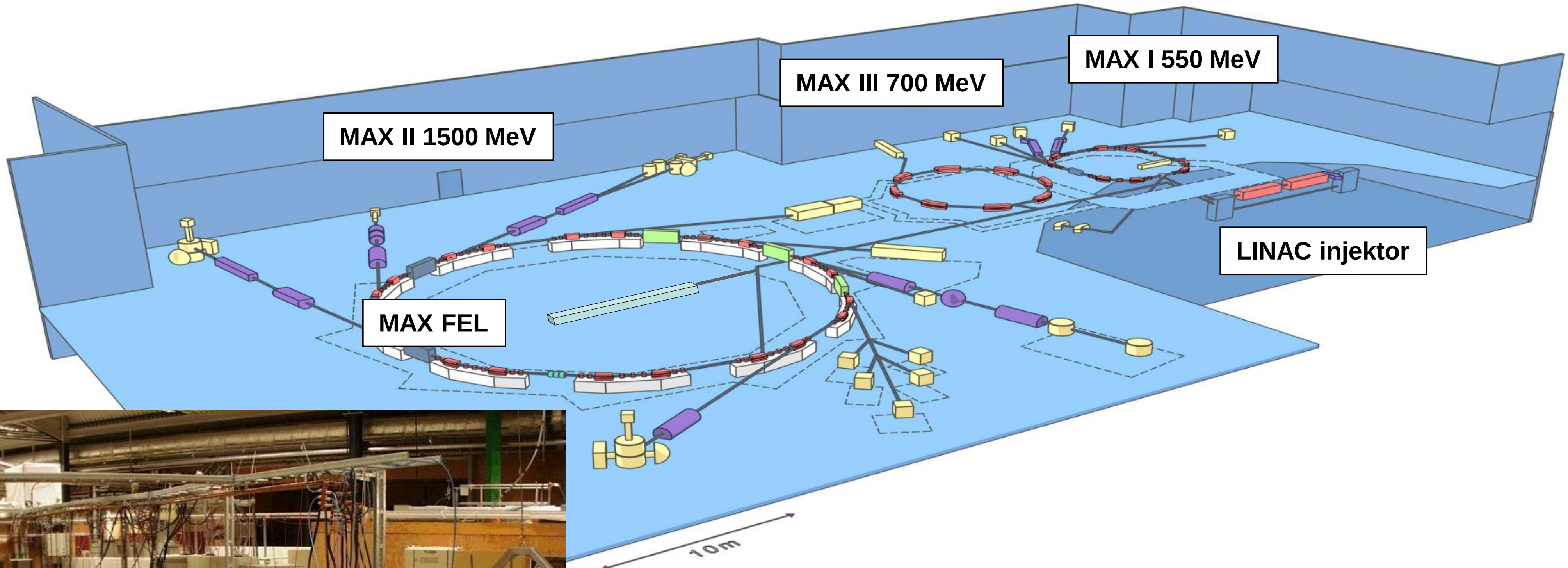


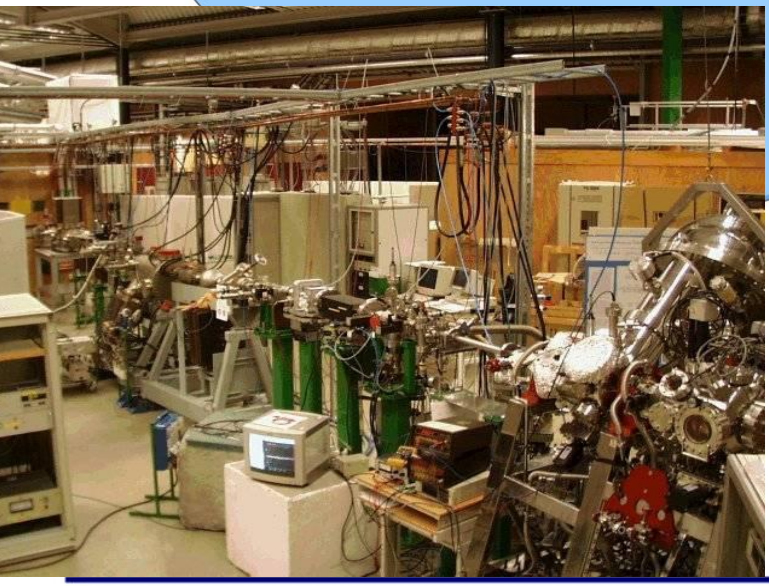


Users at MAX-lab



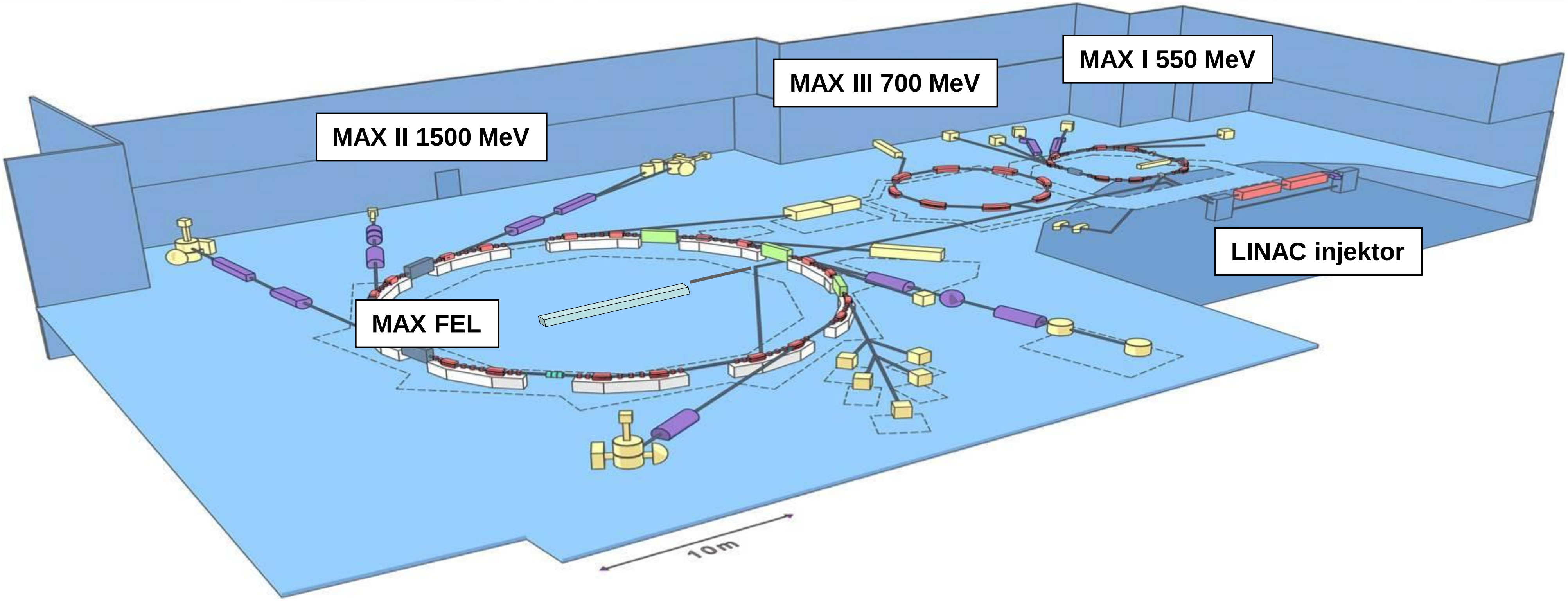
MAX-lab Today – A National Laboratory for Synchrotron Radiation Based Science





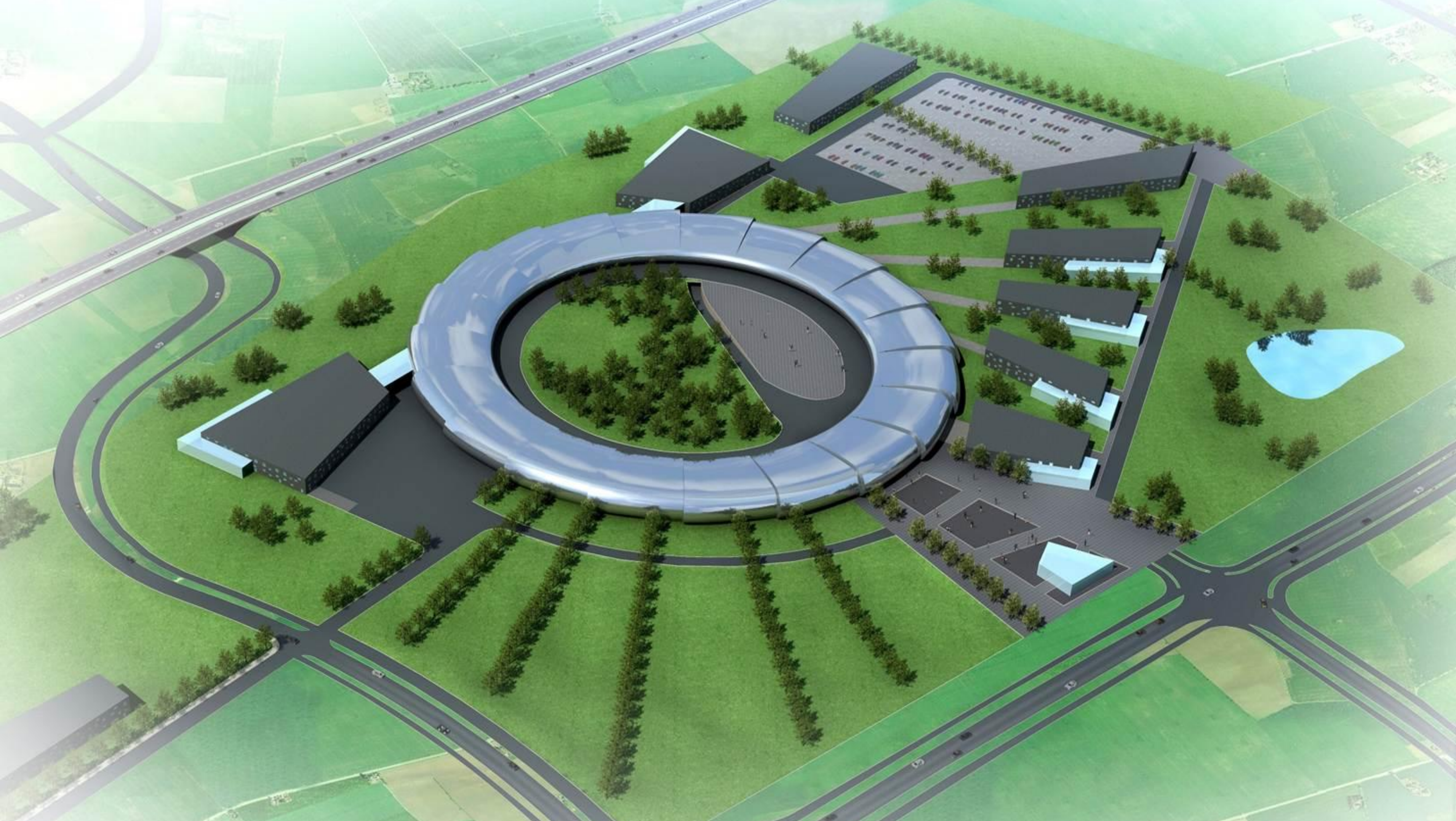
1985 MAX I – Synchrotron Radiation & Nuclear Physics
1997 MAX II – Synchrotron Radiation – higher energies
2008 MAX III – SR – lower energies & Prototype for MAX IV
2009 MAX-FEL – Test Facility for Free Electron Laser
(EUROFEL – IRUVX)

MAX-lab Today – A National Laboratory for Synchrotron Radiation Based Science



→ 3 Storage Rings in operation
> 20 Beamlines (experimental stations) in operation
> 850 Annual Users
Open 41 weeks / year

MAX IV



MAX IV – Past

2002 – 2006

Dialogue with the user community

First funding (KAW)

Conceptual Design Report (CDR)

2006 – 2008

Evaluation(s)

Redesign(s)

Continued dialogue with user community

2009

Research Government-Bill

27th of April
MoU between Research Council, Vinova, LU & Region of Skåne. Secured funds for a “start version” of MAX IV.

MAX IV Present & Future

2009

City plan for the MAX IV area.

Procurement procedure building company

2010

Detailed drawings

First orders

22 Nov
Ground Breaking Ceremony

2010 – 2015

18 May 2011- construction started!

2013 Linac

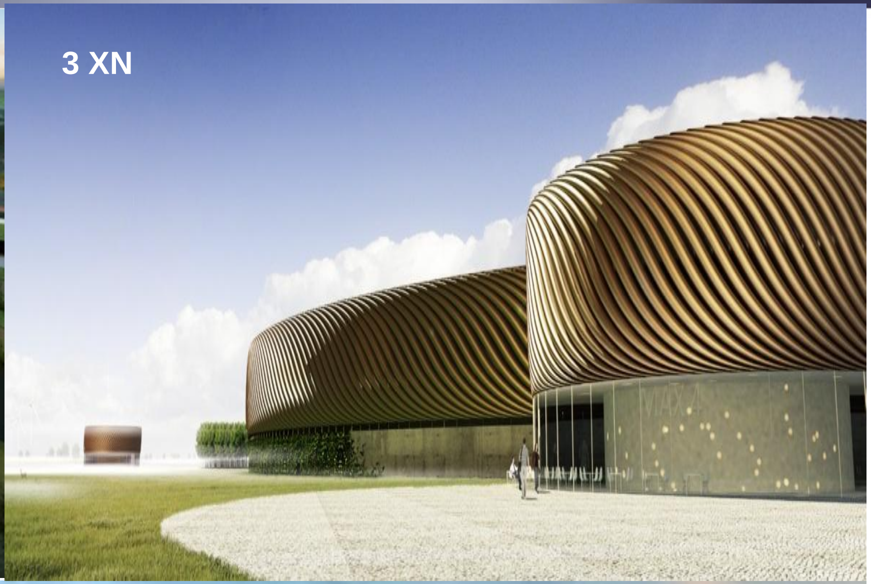
2013 Building (rings)

2015 1^{st} beam

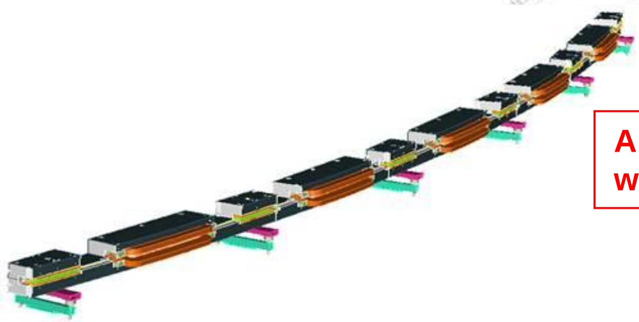
2016

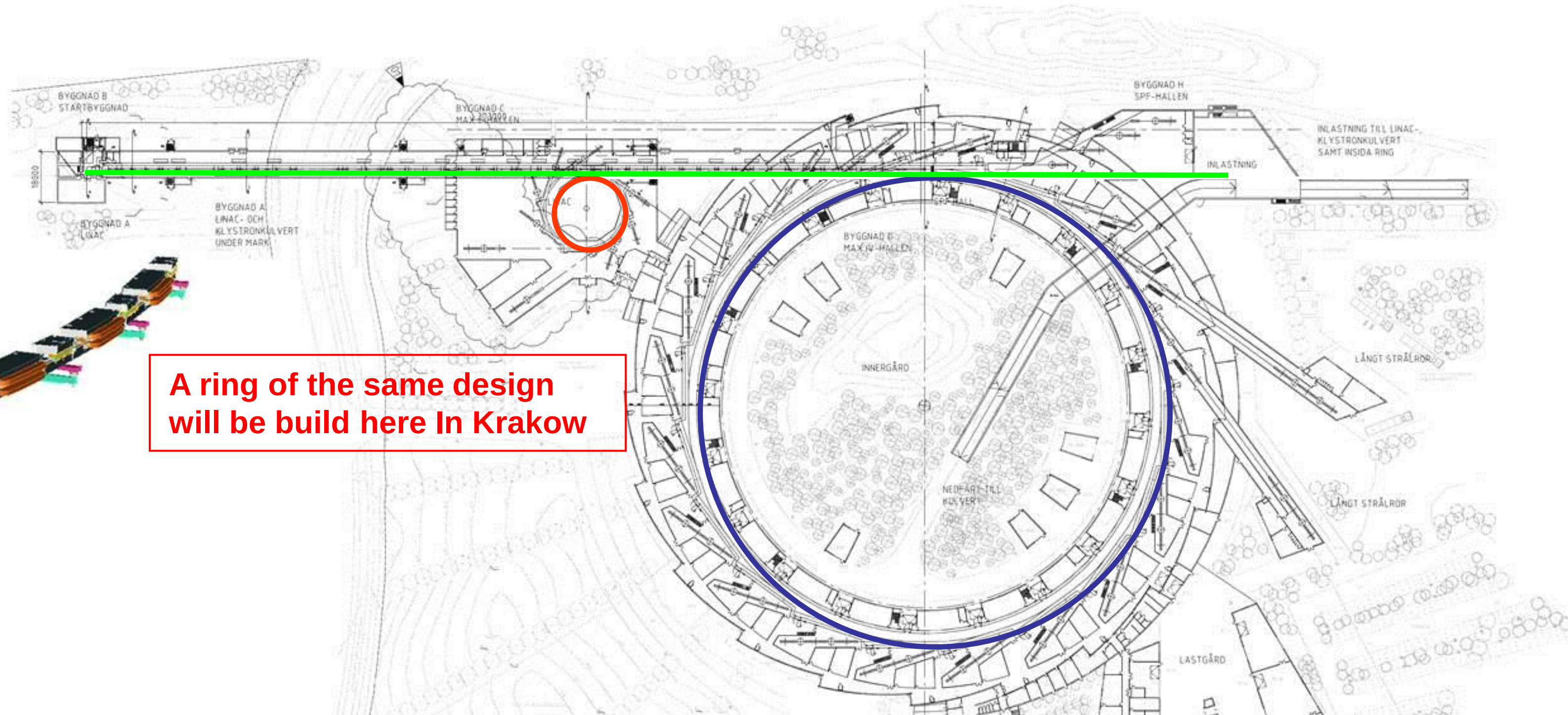
Start version of MAX IV in operation

Building?



MAX IV – Unique Design





3 GeV ring	20 straight sections (0.24 nmrad)
	528 m in circumference
1.5 GeV ring	12 straight sections (5.6 nmrad)
	96 m in circumference (≈ MAX II)
3 GeV linac	Injections + Short Pulse Fascility (partly underground)

MAX IV - A state-of-the-art storage ring!

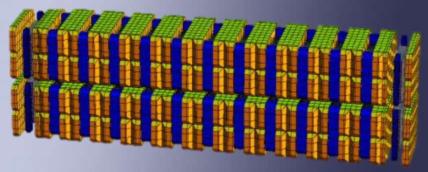
New Facilities In Europe

Facility	Place	Year	Emittans
ELETTRA	Trieste	1993	7-9.7
ESRF	Grenoble	1994	4
MAX II	Lund	1997	8.8
BESSY II	Berlin	1998	5.2
SLS	Villigen	2001	5
SOLEIL	Paris	2007	3
DIAMOND	Oxford	2007	2.74
PETRA III	Hamburg	2010	1
MAX IV	Lund	2015	0.24

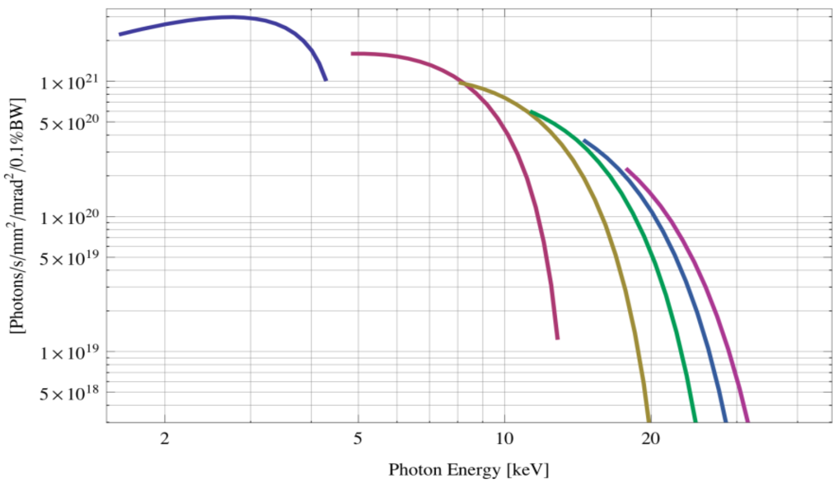
US

Facility	Place	Year	Emittans
NSLS II	Brookhaven	2015	0.6-1

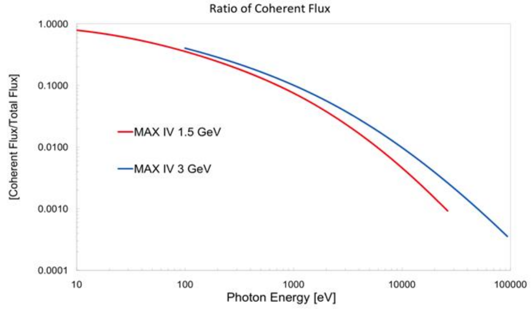
Emittance => Brilliance & Coherence



Brilliance of the pmuA ID



Coherent fraction for MAX IV

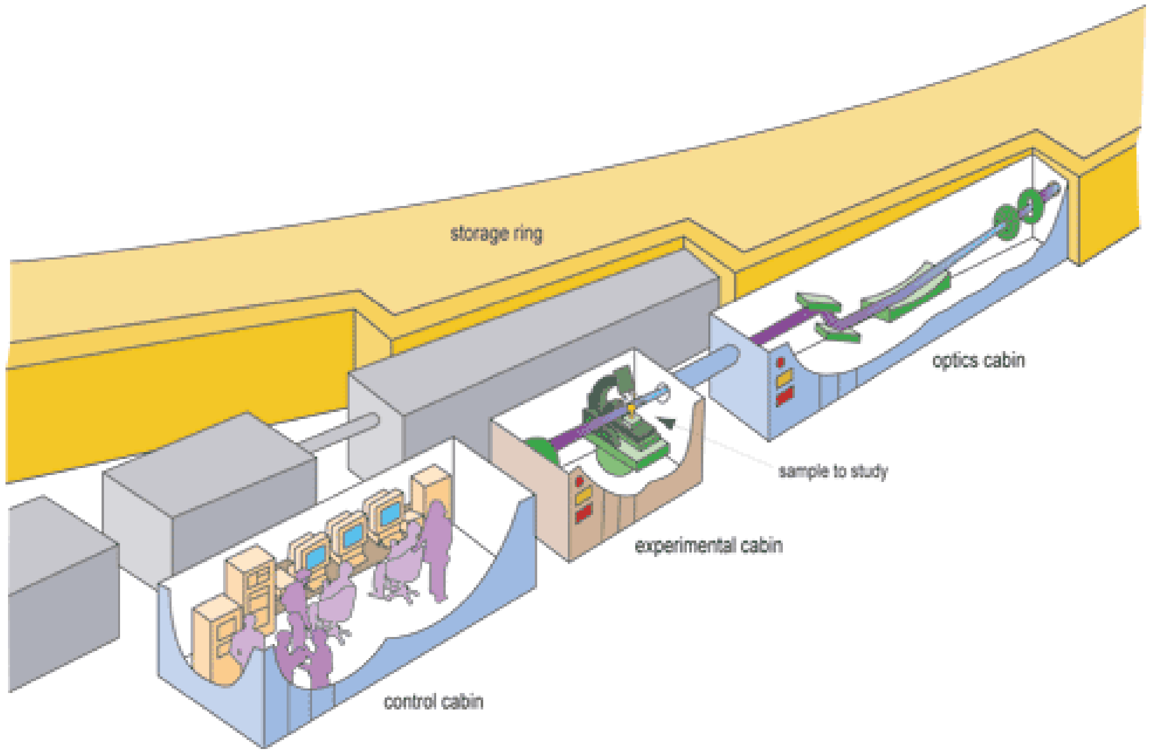


MAX-lab

Example: The In-vacuum undulator pmuA

Period	18.5	mm
Gap	4.2	mm
Peak Field	1.241	T
Effective Field	1.111	T
Peak k-value	2.145	
Effective k-value	1.920	
Higher Order Contr.	10.33	%
Maximum e-beam deflection	0.32	mrad
Electron Beam Energy	3.0	GeV
Electron Beam Current	500	mA
Max Critical Energy	7.429	keV
Emitted Power	13.306	kW
Photon Energy, n = 1	1.625	keV
Total Length	3783.3	mm

The Beamlines



The Process

27th of April 2009	**Funding for a start version of MAX IV secured – not including beamlines**
Spring 2010	**First evaluation:** **10 beamlines proposals were selected out of 30 (!) different beamline proposals.** **Conceptual design studies including budget and required staffing.**
Spring 2011	**Second evaluation:** **International referees, National Reference Group, MAX-labs Program and Science Advisory Committees & the MAX-labs directorate.**
1st of May	**A proposal on a first phase beamline program including a list with 7 beamlines submitted to KAW. For *partial* funding from KAW**
Summer 2011	**Co- financing?** **Staffing**

The 7 Beamlines

Prioritization criteria: **Utilizing the MAX IV performance**

Most beneficial for the Swedish Research Community

1. **A multipurpose high throughput beamline for macromolecular crystallography**
2. **VERITAS – a beamline for soft X-ray resonant inelastic X-ray scattering**
3. **HIPPIE – a high pressure and high resolution electron spectroscopy beamline**
4. **NANOMAX - a hard X-ray nanoprobe beamline at MAX IV**
5. **SPF – A hard X-ray beamline at the short-pulse facility**
6. **ARPES – a beamline for angle resolved photo electron spectroscopy**
7. **XAS – a beamline for in-situ hard X-ray spectroscopy**

Other initiatives for 1st phase beamlines (founding outside KAW)

E.g.

- **Biomedical beamline**
- **(Danish) crystallography beamline**

1 Protein Crystallography

Impact of synchrotron radiation on structural biology

Frontiers in macromolecular crystallography

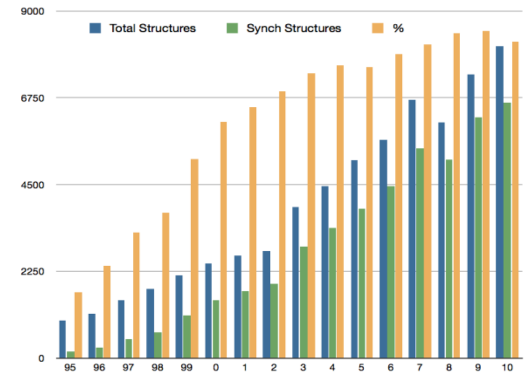
- **(Even) smaller crystals**
- **(Even) better resolution - Atomic molecular structure - resolution down to < 1.0 Å**
- **(Even) more complex structures - No size limit: very large complexes in relevant functional states can be studied, e.g. organelles (the ribosome), multi-subunit DNA and RNA polymerases, very large viruses**

SMALLER, STRONGER & MORE PARALLEL BEAM

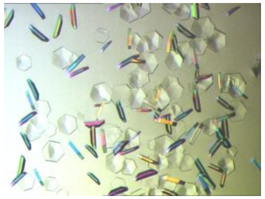
….. and you need to find the best possible crystal

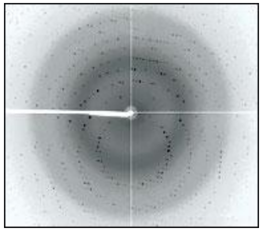
Partly solved by scanning more candidates and thereby finding the best crystal to improve the overall quality of the data collected.
More challenging structural biology problems are being solved more rapidly and with higher quality.

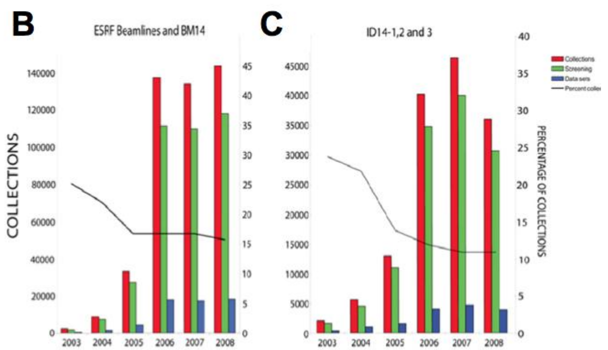
AUTOMATION



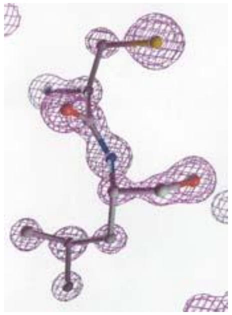
 # new X-ray structures solved

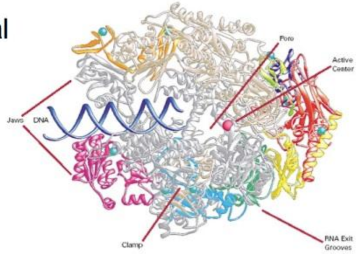






Green screening; Blue collected; Red total

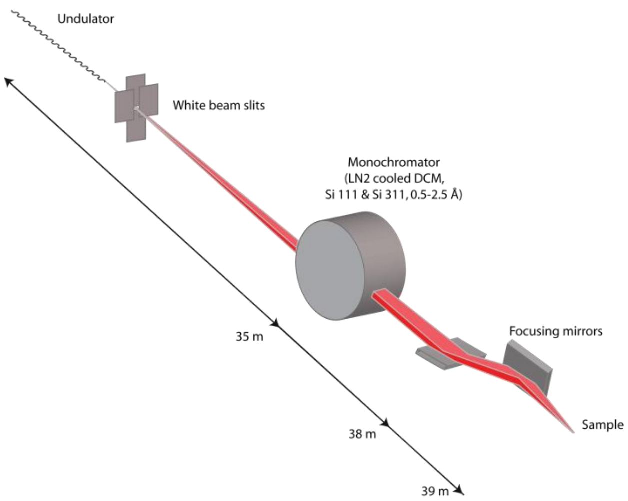




The impact of automated sample-changing technologies on data-collection at the ESRF.

1 Protein Crystallography

“A world-class production facility with high throughput and near microfocus performance suitable for large unit cells”



“A simple optical design that yet takes full advantage of the unique properties of MAX IV”.

Challenge: a turn over time of < 2 minutes
- **Goniostat 90° /sec, positional error ±2mDeg , SOC < 1µm**
- **Detector: shutter less measurements**
- **Robotic sample loading (option for remote data collection)**

Challenge: variable focus 100 to 10 µm
- **DCM with vertical rot. axes for improved mechanical stability**
- **Removable bimorph mirror with a slope error of < 0.2 µrad**

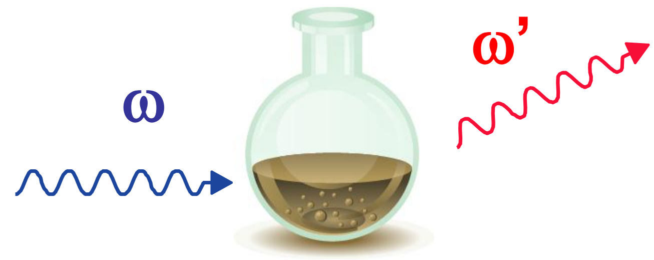
PX_HT – a multipurpose high throughput beamline for macromolecular crystallography

Photon Source	18.5 mm period in-vac U (2m)
Spectral Range	5 – 25 keV
Optics	liq N_2 DCM, Adaptive KB-mirror (Si, Rh, Pt strips)
Spot size	20 *10 – 100*100 µm (H*V)
Flux	> 10^{13} ph/s
Exp. Techniques	Protein crystallography with MAD & XAFS capacity

Spokespersons: Gunter Schneider Karolinska institutet, Richard Neutze Gothenburg University

2 VERITAS

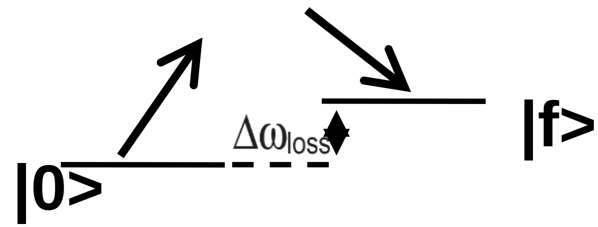
VERITAS – a beamline for soft X-ray resonant inelastic scattering (RIXS)



<u>RIXS</u>

Photon in – photon out
Inelastic scattering process (energy is not conserved)
The X-rays causes electronic excitations (tune the energy to abs. edge)I
Determine the energy and momentum of the emitted photons

Provides information about the excitation stages (core holes)



Studies of the electronic structure in complex materials

Some (ex)samples: **Battery research (e^- structure *in-situ*)**
Molecular biology (RNA – metal ions) – UHV not required
High Tc superconductors
Magnetic properties

$$\omega - \omega' = \Delta\omega_{\mathrm{loss}}$$

$$\Delta\omega_{\mathrm{loss}} = \omega_{\mathrm{vib}} + \omega_{\mathrm{elec}}$$

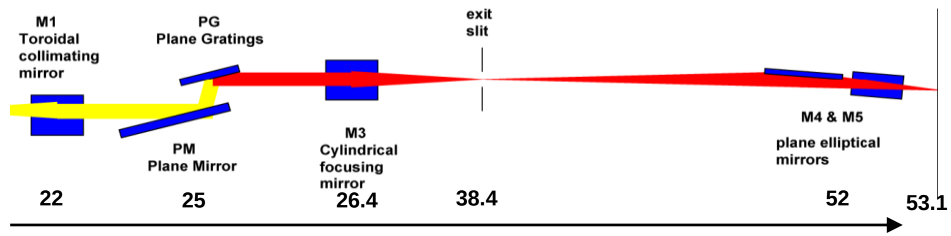
<u>Requirements</u>

- **Small cross section (weak process) > high brilliance**
- **High spatial and energy resolution (E/ΔE of >50.000 at 500 eV).**
- **Polarized X-ray beam**

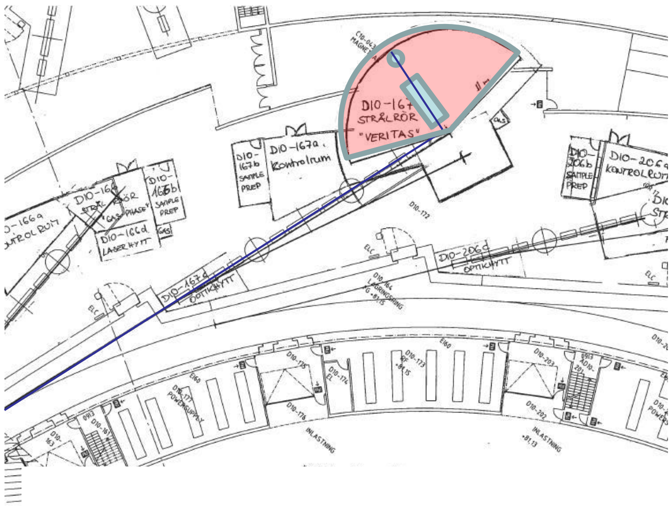
2 VERITAS

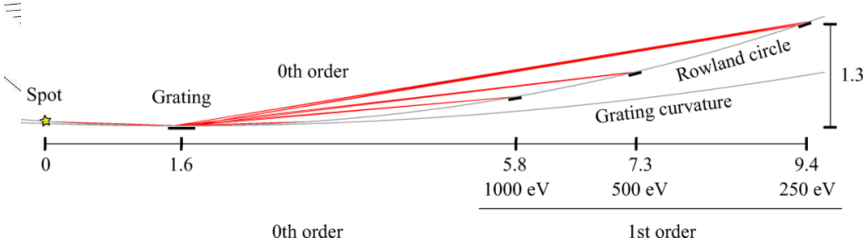
Design goal: Produce higher resolution and higher photon flux that any existing or foreseen beamline in the energy range of 275 – 1500 eV.

Resolving power of the beamline 50 000 should be matched of the spectrometer



Preliminary beamline layout (Sankari 2009)





VERITAS – a beamline for soft X-ray resonant inelastic scattering (RIXS)

Photon Source	EPU (3 GeV)
Spectral Range	275-1500 eV (1 st harmonic)
Optics	Collimated Plane Grating Monochromator (PGM) with refocusing optics.
Spot size	1*1 μm
Resolving Power	50 000@ 500eV (>10^{12} ph/s)
Exp. Techniques	RIXS

3 HIPPIE - High pressure and high resolution electron spectroscopy

X-ray photoelectron spectroscopy (XPS)

Photon in (soft X-rays 200-2000 eV) – electron out

A quantitative technique where the energy levels of core level electrons are studied
Information on elemental composition, empirical formula, chemical state and electronic state of the elements.

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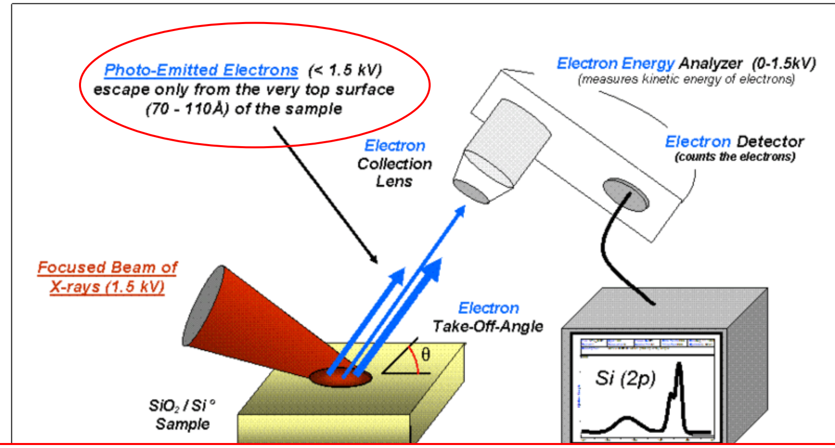
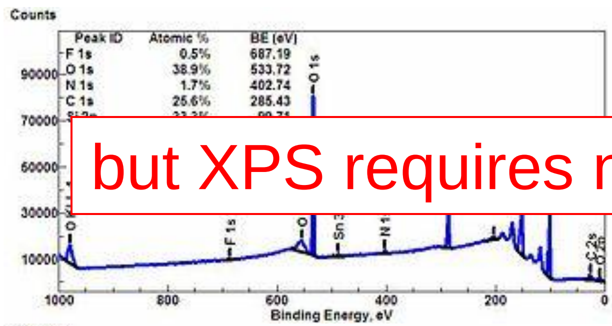
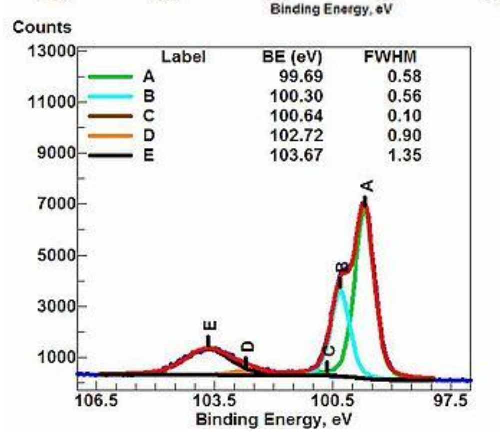




but XPS requires normally ultra high vacuum (UHV) conditions



High Resolution Spectra (Si(2p))

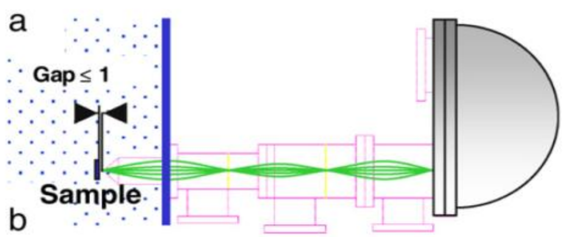
Kai Siegbahn (1918-2007)
Nobel Prize in 1981 for developing this technique which he referred to as Electron Spectroscopy for Chemical Analysis (ESCA), since the core levels have small chemical shifts depending on the chemical environment of the atom which is ionized, allowing chemical structure to be determined.

VG SCIENTA
a gammadata company

MAX-lab

3 HIPPIE - High pressure and high resolution electron spectroscopy

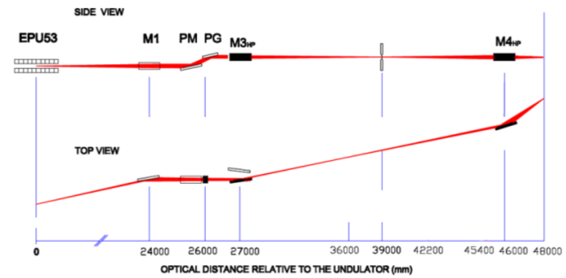
Beamline at 3 GeV ring for near-ambient pressure X-ray photoelectron spectroscopy



H-P set-up, maximum pressure: ~10 to 25 mbar
Differential pumping + electrostatic lenses

HIPPIE will serve a user community much wider than the traditional electron spectroscopy community by offering the following *dedicated high pressure cells for in-situ measurements:*

- **Catalysis and Corrosion studies (surface – gas)**
- **Liquids**
- **High temperature treatment**
- **Biological samples**



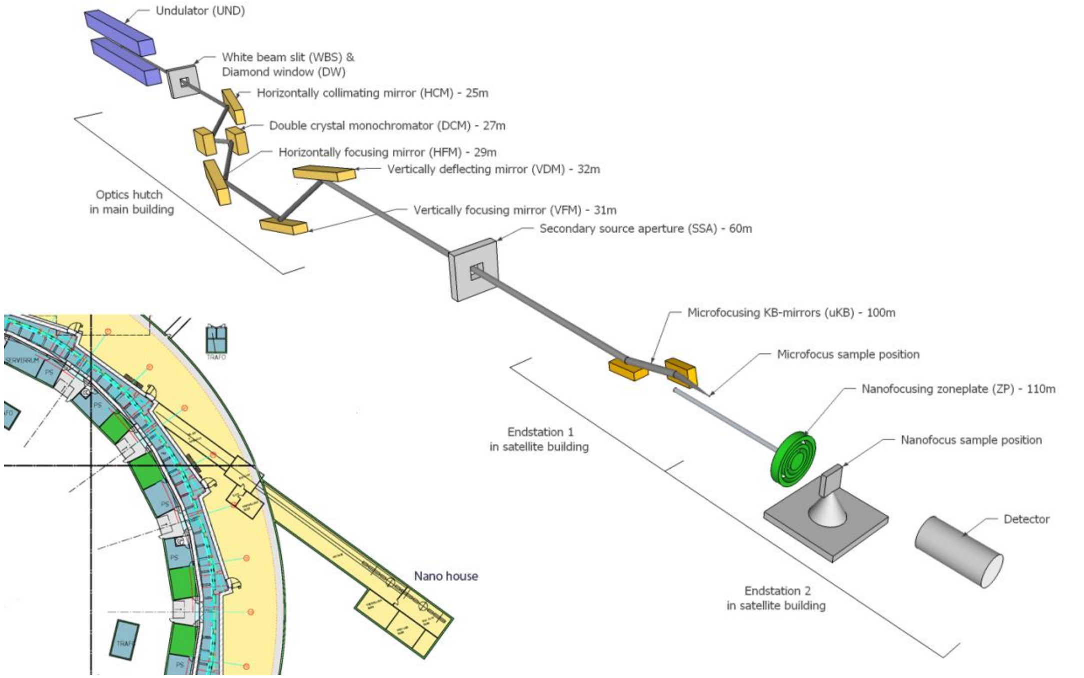
HIPPIE – High Pressure and High Resolution Spectroscopy

Photon Source	EPU53p0 (3 GeV)
Spectral Range	270-2000 eV (1 st harmonic)
Optics	Collimated Plane Grating Monochromator (PGM) with refocusing optics.
Spot size	50 * 50 μm
Exp. Techniques	

High Pressure (25 mbar) Photoelectron Spectroscopy

Spokesperson: Joachim Schnadt, Lund University

4 NANOMAX



The NANOMAX building extending 104 m from the source

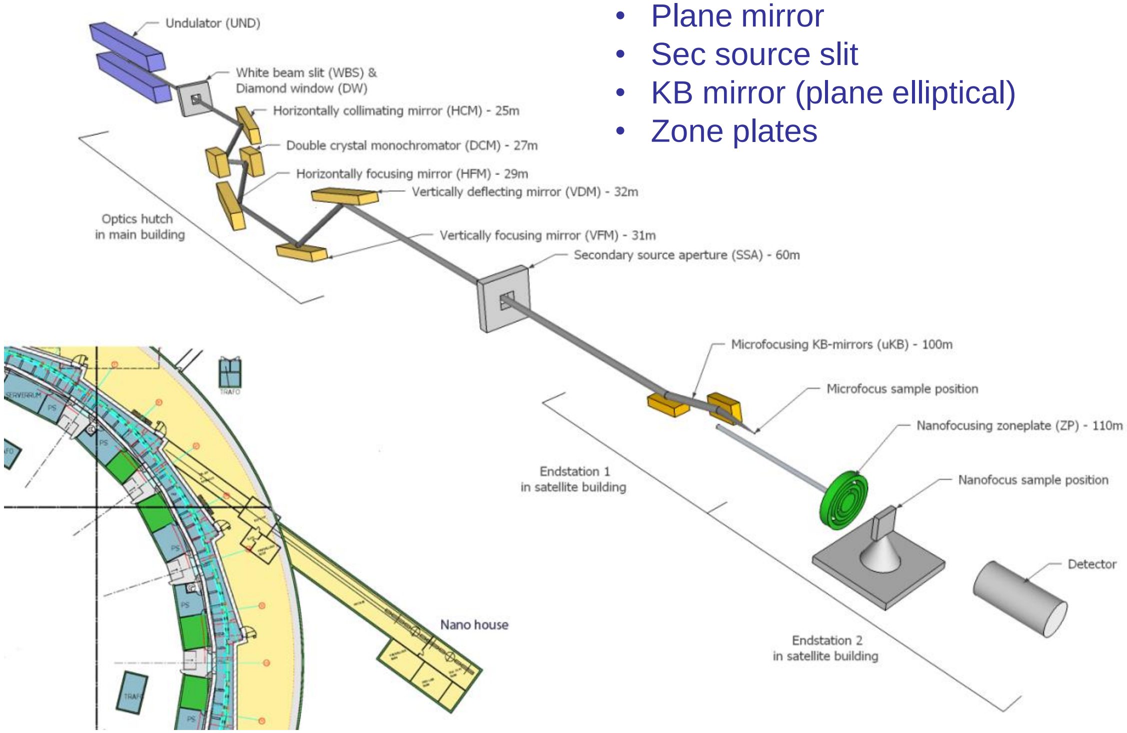
NANOMAX - a hard X-ray nanoprobe @ MAX IV

Photon Source	18.5 mm period in-vac U (2m)
Spectral Range	5 - 30 keV
Optics	4 mirrors images the primary source onto a pair of secondary source slits @ 60 m. liq N_2 cooled DCM monochromator 1 KB mirror 2 Zone plates
Spot size & Flux	Endstation 1 > 300 nm, $2 \cdot 10^{12}$ ph/s @ 10 keV Endstation 2 30 – 50 nm, $5 \cdot 10^{10}$ ph/s @ 10 keV
Exp. Techniques	Scanning X-ray Microscopy (SXM) (coherent) imaging, scattering (XRD & SAXS), XRF

Spokespersons: Ulrich Vogt, Royal Institute of Technology, Ulf Johansson, MAX-lab, Anders Mickelsen, Lund University

4 NANOMAX

• In-vacuum undulator	5 – 30 keV
• Front end	50 μrad, filter
• Horizontally collimating mirror	& heat load
• DCM (vertical rotation axes) Si(111)	
• Hor. focusing on the sec source slit	slope error 0.5 μrad rms
• Vert. focusing on the sec source slit	slope error 0.2 μrad rms
• Plane mirror	parallel beam, harmonic rejection
• Sec source slit	beam size 100*20 μm, slit smaller
• KB mirror (plane elliptical)	microfocus station
• Zone plates	nanofocus station

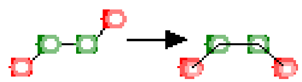


5 The Short-pulse facility (SPF)

”Ultrafast Science”

Chemical/ structural dynamics with the fundamental timescale set by the X-ray pulses matching those of a molecular vibrations ~100 fs

Ultrafast phase-transitions

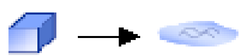


E.g.

- structural changes in ferroelectric memories
- Laser melting of ice

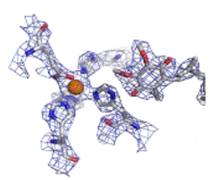
Ultrafast chemical reactions

- Monitor the three-dimensional evolution of a molecular system in the course of a chemical reaction

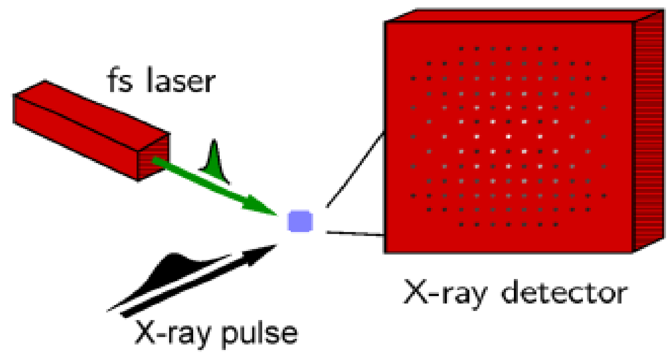


Ultrafast bio-chemical reactions

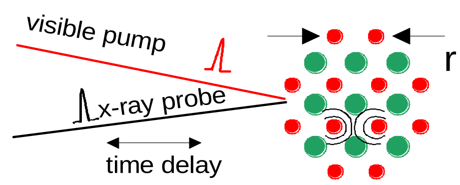
- Photo biology

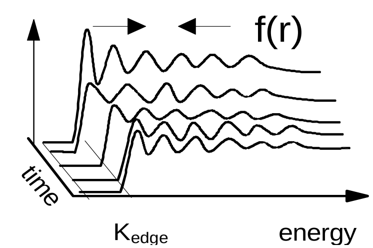


Time-resolved X-ray scattering (XRD & SAXS)



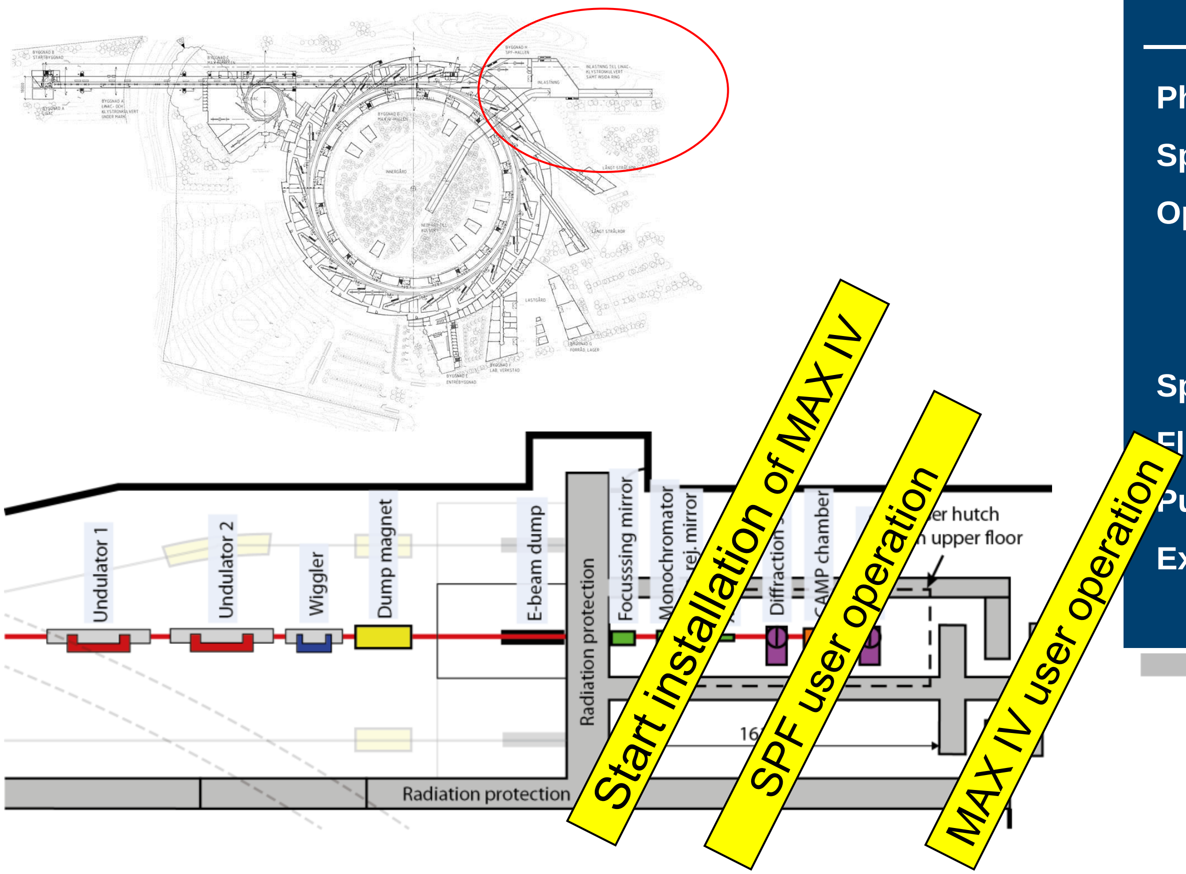
Time-resolved EXAFS





5 SPF (Short Pulse Facility)

No odd filling patterns of the ring these are optimized for average intensity but the linac …



2011	2012	2013	2014	2015	2016	2017	2018

SPF

Photon Source(s)	in vacuum und (10m?) & wiggler
Spectral Range	1.8 – 30 keV
Optics	DCM Si(111) & InSb(111) + ML mirror + white beam option.
Spot size	0.2*0.2 mm^2 (unfocused)
Flux	10^{7-8} ph / pulse (100 Hz)
Pulse duration	100 fs
Exp. Techniques	X-ray Scattering dispersive EXAFS

Spokesperson: Jörgen Larsson, Lund University

6 ARPES

(10 – 1000 eV) Photon in – (Valence) electron out

Measure the kinetic energy and angle (momentum) of the photo electrons

Detailed information on the electronic structure ("new materials")
- **Nanoelectronics – graphene**
- **Magnetic semiconductors**

Well ordered samples

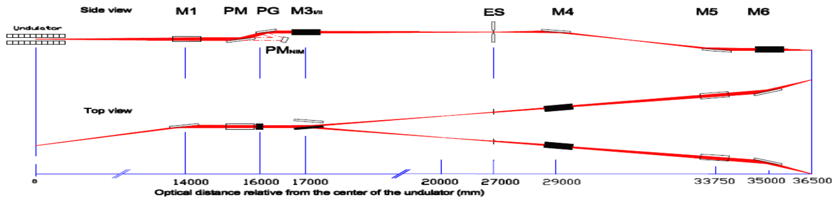
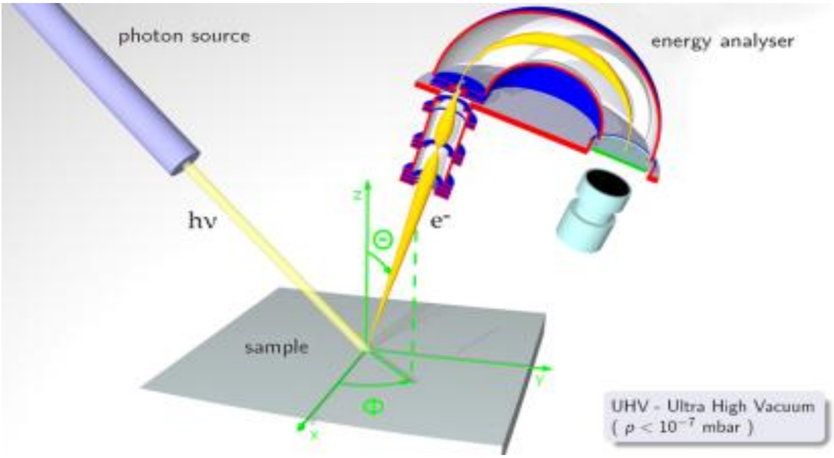


Figure 2. Optical layout of the ARPES/Spin-ARPES beamline.

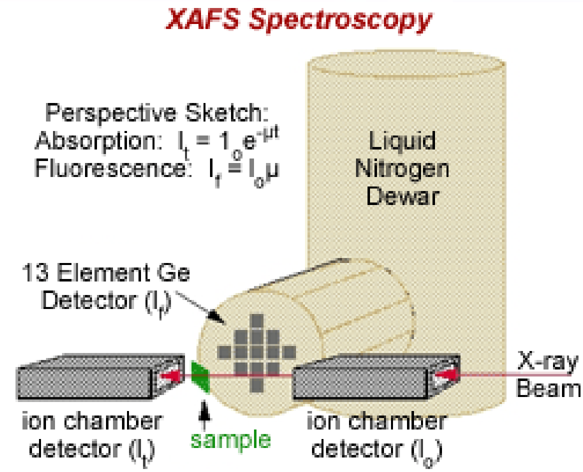


ARPES – a beamline for angle resolved photo electron spectroscopy

Photon Source	EPU 84 (1.5 GeV)
Spectral Range	10-1000 eV (1 st harmonic)
Optics	Collimated Plane Grating Monochromator (PGM) with NIM option Refocusing optics.
Spot size	25*25 μm
Resolving Power	100 000@ <100eV (>10^{12} ph/s)
Exp. Techniques	ARPES/ option spin-ARPES

Spokesperson: Roger Uhrberg, Linköping University

7 *In-Situ* XAFS Spectroscopy Beamline

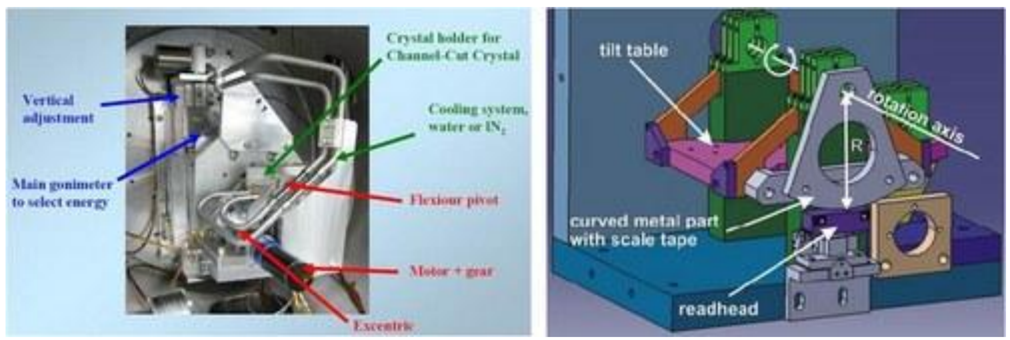


XAFS spectroscopy is element specific technique, and can give local information including oxidation state and speciation, electronic and structural information.
EXAFS & NEXAFS & XRF

- Sensitive (ppm range)
- No sample prep
- Can detect the element of interest in any phase or form

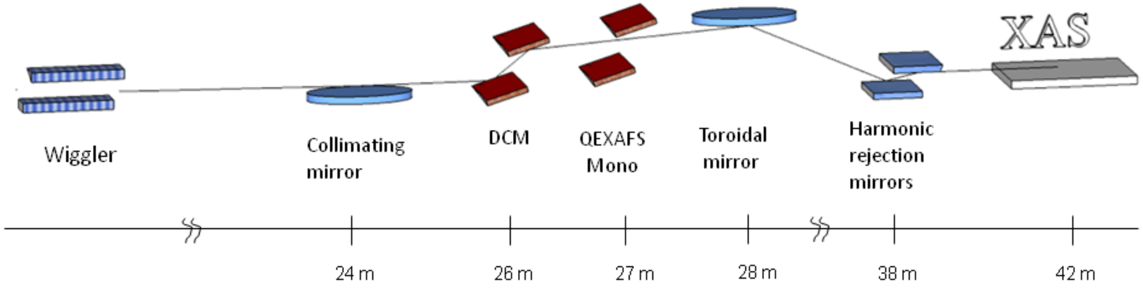
- Slow (from seconds – to hours)
- Stability

Quick Scan Monochromator (QEXAFS)
Channel-cut crystal mounted to a CAMdrive
tilt table for rapid angular oscillations. The monochromator is able to record full EXAFS spectra in less 50 ms & 12 ms for a XANES spectra



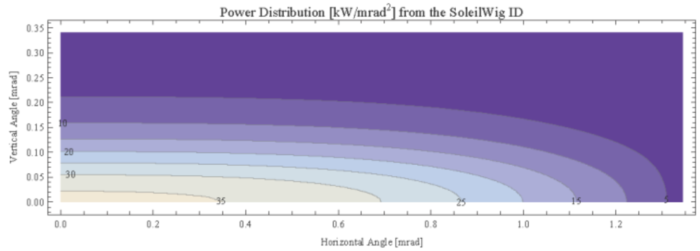
Developed by Prof R Frahm, University of Wuppertal (Germany).

7 *In-Situ* XAFS Spectroscopy Beamline



The QEXAFS option requires white radiation (wiggler or bending magnet beamline).

HEAT LOAD



Total Power 21 kW (Power Density 35 kW/mrad^2)

Sample 65 mW

Heat Absorbers, slits: 200W/mm^2 (Cu 10)
Mirror: absorbs 1 kW - stability
Mono 700 W (1 m^3 liq N_2) – stability

Hard X-ray Environment XAS

Photon Source	38 period 2.1 T wiggler
Spectral Range	4 – 40 (or 50) keV
Optics	Fixed angle collimating mirror, DCM & QEXAFS mono, toroidal + harmonic rejection mirror.
Spot size	Tunable 1 x 1 mm^2 to 3 x 18 mm^2
Exp. Techniques	XAS (EXAFS; XANES, XRF & QEXAFS)

Spokesperson: Ingmar Persson, Swedish Agricultural University

The 7 Beamlines

1. A multipurpose high throughput beamline for macromolecular crystallography
2. VERITAS – a beamline for soft X-ray resonant inelastic X-ray scattering
3. HIPPIE – a high pressure and high resolution electron spectroscopy beamline
4. NANOMAX - a hard X-ray nanoprobe beamline at MAX IV
5. SPF – A hard X-ray beamline at the short-pulse facility
6. ARPES – a beamline for angle resolved photo electron spectroscopy
7. XAS – a beamline for in-situ hard X-ray spectroscopy

23 More to go!

MAX IV & ESS