Updated Science Case – SoftiMAX

Facts

Title	SoftiMAX (https://www.maxiv.lu.se/accelerators-beamlines/beamlines/softimax/)
External collaborations	MAX IV-Soleil (Sextants, Hermes), Uppsala (Maia, Dürr, Agåker), KTH (Vogt), PSI (Rössner, David), Uni. Tübingen (Obst), T. Tyliszczak, CLS (R. Berg)
Original budget and funders	94.4 MSEK, Vetenskapsrådet
Official start	April 2014
Expected date of completion	Spring 2020 (first light: late 2019) for STXM branch, 2021 for CXI

Introduction to the project

The SoftiMAX beamline exploits the best of the brilliance of MAX IV: coherent soft X-ray microscopy using either a nano or micro beam to push the boundaries of resolution. The Scanning Transmission X-ray Microscopy (STXM)/ptychography branch will provide spectroscopy and phase maps (≤10 nm resolution) for many different scientific fields, ranging from e.g. environmental science to magnetism, catalytic chemistry, and the life sciences. The Coherent X-ray Imaging (CXI) branch will aim at studying materials and magnetic samples using Fourier transform holography and (magnetic) X-ray resonant scattering. This branch can also be used for time-dependent measurements to study dynamics in materials and life science samples. SoftiMAX will moreover provide an excellent platform for developing novel techniques using highly coherent beams on the nanometer (point probe) or micrometer (full field) scale.

Technical description of the project

Energy range 275 – 2500 eV, full polarisation control, focus diameter: 10-100 nm (STXM/ptycho) / 20 micron (CXI). Flux: up to 10^{11} in a diffraction limited spot (25 nm ZP, STXM/ptycho), up to 5×10^{13} in a 20 μm^2 spot (CXI).
Sample environment (STXM/ptycho): vacuum chamber with fast fly scan stage & point detector (MHz, STXM), fast 2D detector for ptychography (around 100 frames/s), possibility for different sample environments (e.g. hydrated, electrochemistry, local magnetic field), fluorescence detector.
Sample environment (CXI): UHV chamber with in-plane goniometer, small pixel-high dynamic range 2D detector, thermostat (<20K), and magnetic sample environment (≤ 1T)

Technical implementation:
EPU (48mm period, 11 mm min_gap, collimated plane grating monochromator (330 l/mm, 1200 l/mm), zone plate refocusing (STXM/ptycho), Rh-Au coated mirrors (STXM), KB refocusing (CXI),
CCD with fast read-out speed (STXM/ptycho), large CCD with low read-out noise, small pixel size (CXI), direct data pipeline to parallel computing cluster.

Present status of the project

Optics: installed, awaiting final alignment and baking (Kirkpatrick-Baez mirrors (KB) system in pre-procurement phase, 300 l/mm grating pending).
Infrastructure: BL vacuum infrastructure is under construction, electrical/water/internet installation nearly completed, gas systems awaiting installation. IT & PLC: in queue
Undulator: installed. Front end: installed.
STXM/ptycho end station: ordering and assembly phase. CXI end station: early design phase.
Data analysis: (with NanoMAX & IT-group) towards 2D ptychography tests.

Expected status end 2019

The beamline with the STXM/ptycho branch: in early commissioning. The CXI branch: KB mirrors on order, end station in production phase.

Major partners and additional funding

The MAXIV-SOLEIL project has funded sample environments for the STXM and CXI side, as well as a 2D camera. Zone plate development is done in collaboration with B. Rössner & C. David (PSI) and U. Vogt (Biox, KTH). Data analysis/handling will hopefully benefit from a grant proposal involving MAX IV, Uppsala (F. Maia: Advisory Board SoftiMAX) and others. A control system for the STXM is developed by T. Tyliszczak, formerly ALS, and a follow up is done with R. Berg (CLS). A grant from VR funds a 50% position in sample preparation of life science samples for imaging/spectroscopy. The CXI endstation is co-designed with H. Dürr, M. Agåker (Uppsala). A Röntgen-Ångström collaboration funds a post-doc at SoftiMAX for magnetic measurements. M. Obst (Uni. Tübingen) assists environmental science users with sample preparation and sample holder advice.

Changes made since the start of the project

Recruitment of a second scientist (CXI) has taken 1.5 year: the CXI branch is therefore behind the STXM/ptychography side in maturity. CXI has expanded to include both transmission and reflection experiments. Appropriate tools for coherence evaluation had to be developed simultaneously with the detailed optical design (K. Klementiev, MAX IV Laboratory). Intensities at STXM/ptycho imply faster scanning than currently (commercially) available and faster 2D detectors would also be needed. In this regard, the first STXM station is developed in house with T. Tyliszczak for speed optimisation, at the expense of LN2 cooling, which will be the focus of the second stage, or STXM-II.

Comparison to similar beamlines world wide

CSX-1 at NSLS II (USA) (https://www.bnl.gov/ps/beamlines/beamline.php?b=CSX-1)
SEXTANTS, HERMES at SOLEIL (France) (http://www.synchrotron-soleil.fr/Recherche/LignesLumiere/HERMES)
ID08 at Diamond Light Source (UK) (http://www.diamond.ac.uk/Beamlines/Spectroscopy/I08)
SM at CLS (Canada) (http://exshare.lightsource.ca/sm/Pages/SM-Home.aspx)
11.02/5.3.2.1/Cosmic at ALS (USA) (https://www-als.lbl.gov/index.php/beamlines/beamlines-directory.html)
MAXYMUS at Bessy (Germany) (https://www.helmholtz-berlin.de/quellen/bessy/instruments-photons/index_en.html)
Pollux at SLS (Switzerland) (https://www.psi.ch/sls/pollux/)
Twinmic at Elettra (Italy) (https://www.elettra.trieste.it/it/lightsources/elettra/elettra-beamlines/twinmic/twinmic.html)

How do you see that the project could develop beyond 2023?

The unprecedented coherent flux will give rise to observing smaller effects (e.g. magnetic, orbital) and push the boundaries of resolution (towards 1 nm in ptychography) and become more turnkey, easily useable even for inexperienced users. Simultaneously, the intense beam will allow new coherent techniques to be developed.

The energy range of the beamline can be expanded to 3 or 4 keV, and optimised by purchasing a multilayer grating.

A second end station can be added to either the STXM/ptycho and CXI branches to tailor more specifically to the high or low energy range/new coherence techniques/specific scientific areas, such as strong magnetic fields/bio-imaging/3D-tomography/time-resolved (laser, beam chopper) - it remains to be seen which scientific areas will come to dominate the user community at SoftiMAX. This could also include building a second STXM/ptycho station focused on cryosamples.

Crucial to stay at the forefront in all areas are the 2D detectors, which will have to be replaced with newer models after a number of years in service.

Zone plate development and production: with Vogt (Biox,KTH) and Rössner/David (PSI) especially important for the tender hard X-ray range and 'special' designs for new coherent techniques. This will require funding in the long term.

We also support a common platform throughout Sweden, *NanoSPAM*, which our Life Science/Soft Matter users can turn to for help in preparing (microtome/ultratome) and characterising (histology, optical microscopy/TEM) their samples before and after beamtime. A similar platform inside MAX IV for material science/surface science, with common peripheral tools is also required.

Data analysis is crucial for indirect imaging methods like ptychography and diffraction-based 3D tomography. Robust algorithms, on-the-fly analysis and fast data transfer are a must. Ongoing efforts with NanoMAX, MedMAX and other relevant (imaging) beamlines are ongoing, together with outside collaborators, like F. Maia (Uppsala). This requires, however, dedicated programming personnel.