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The BALDER Beamline at the MAX IV Laboratory

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The BALDER Beamline at the MAX IV Laboratory

K Klementiev[1], K Norén[1], S Carlson[1], K G V Sigfridsson Clauss[1*] and I Persson[2]

[1]MAX IV Laboratory, Lund University, 22592 Lund, Sweden,
[2]Swedish University of Agricultural Science, Dept. of Chemistry and Biotechnology, 75007 Uppsala, Sweden

E-mail: kajsa.sigfridsson_clauss@maxlab.lu.se

Abstract. X-ray absorption spectroscopy (XAS) includes well-established methods to study the local structure around the absorbing element – extended X-ray absorption fine structure (EXAFS), and the effective oxidation number or to quantitatively determine the speciation of an element in a complex matrix – X-ray absorption near-edge structure (XANES). The increased brilliance and intensities available at the new generation of synchrotron light sources makes it possible to study, *in-situ* and *in-operando,* much more dilute systems with relevance for natural systems, as well as the micro-scale variability and dynamics of chemical reactions on the millisecond time-scale. The design of the BALDER beamline at the MAX IV Laboratory 3 GeV ring has focused on a high flux of photons in a wide energy range, 2.4–40 keV, where the K-edge is covered for the elements S to La, and the L_3-edge for all elements heavier than Sb. The overall design of the beamline will allow large flexibility in energy range, beam size and data collection time. The other focus of the beamline design is the possibility to perform multi-technique analyses on samples. Development of sample environment requires focus on implementation of auxiliary methods in such a way that techniques like Fourier transform infrared (FTIR) spectroscopy, UV-Raman spectroscopy, X-ray diffraction and/or mass spectrometry can be performed simultaneously as the XAS study. It will be a flexible system where different instruments can be plugged in and out depending on the needs for the particular investigation. Many research areas will benefit from the properties of the wiggler based light source and the capabilities to perform *in-situ* and *in-operando* measurements, for example environmental and geochemical sciences, nuclear chemistry, catalysis, materials sciences, and cultural heritage.

1. Introduction

The low emittance 3 GeV ring at the MAX IV Laboratory in Sweden is undergoing commissioning and will be taken in operation in 2016. The BALDER beamline, dedicated to X-ray absorption spectroscopy (XAS) is one of the first phase beamlines under construction and is expected to initiate user operation in second half of 2016. XAS is one of few techniques that will provide detailed molecular information on elements in complex matrices. Very often regarded as a non-destructive technique where a minimum of pre-treatment is required, only very small amounts of material are needed, and concentrations of the studied elements are often low, XAS has become an indispensable tool in research areas such as life sciences, environmental and geochemical sciences and nuclear chemistry, catalysis and materials sciences, and cultural heritage. The design of the BALDER beamline has focused on a high flux of photons in a wide energy range, 2.4–40 keV, with flexibility in beam size and data collection time, and with focus towards implementation of multi-technique analyses on samples.

2. Beamline design

The BALDER beamline requires high flux, broad energy range, high energy resolution, high beam stability and fast energy scanning capability. These requirements are incorporated into the beamline design, which is based on an in-vacuum wiggler source and includes four main optical elements, see Figure 1:

- Vertically collimating mirror with Si and Ir stripes, water cooled
- Double crystal monochromator with Si(111) and Si(311) LN2-cooled crystals
- Toroid focusing mirror with Si and Ir torus
- Harmonic rejection mirrors with Si and Ir stripes (in experimental hutch, not shown in Figure 1)

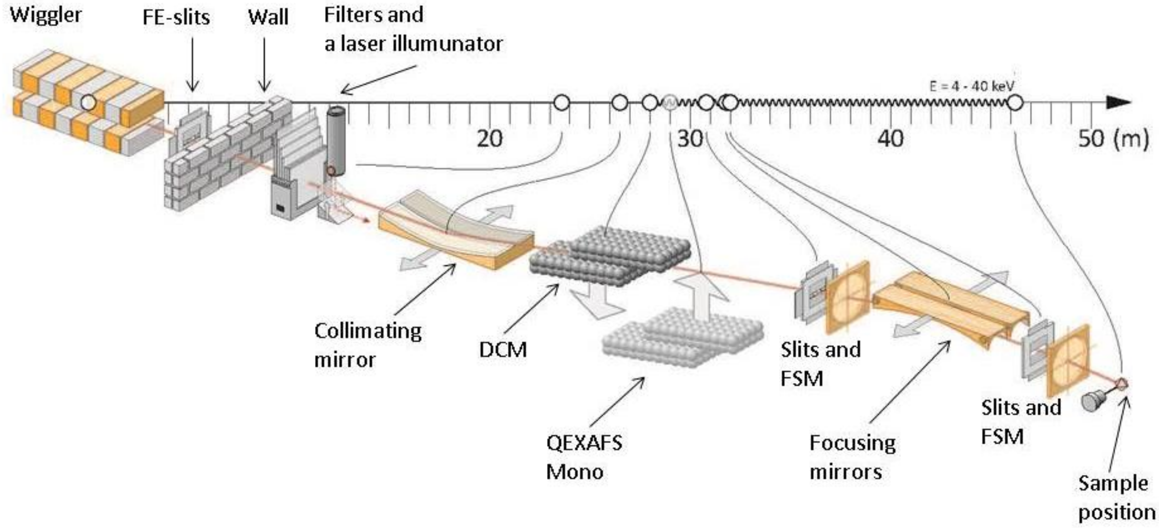

Figure 1. Conceptual optical layout of the BALDER beamline. The “QEXAFS Mono” (quick monochromator) is a possible device for future upgrades.

2.1. The Source

The design concept for the BALDER beamline is based on an in-vacuum wiggler source. The wiggler design of choice is an in-vacuum wiggler developed at SOLEIL. The wiggler is composed of 38 periods of 50 mm producing a magnetic peak field of 2.1 T at a minimum gap of 5.5 mm. The magnetic system consists of a sequence of NdFeB permanent magnets with a magnetic remanence of 1.2 T at ambient temperature [1].

As pointed out by E. Welter [2], a multi-pole wiggler installed at a low-emittance storage ring produces a non-uniform beam. We confirm this statement by using two calculation programs – SPECTRA [3] and xrt [4], see Figure 2.

In order to smoothen the radiation distribution, one can perform tapering – varying the magnetic gap along the wiggler. While SPECTRA is capable of calculating tapered insertion devices, it cannot represent both spatial and energy domains at the same time. We therefore use xrt to study the result of tapering. Low energy radiation is more prone to create the spatial and energy fringes. In Figure 3 we present the most difficult case – the lowest beamline energy, 2.5 keV. For an energy band of 200 eV, one can see the chromatic fringes in the spatial distribution and a non-uniform energy distribution. Both features are gone as one gradually increases the tapering up to 2% (in Δgap/gap). At higher energies, tapering can be smaller, e.g. down to ~0.5% at 9 keV. Moreover, inevitable random errors in the alignment of magnetic poles facilitate the smoothing both in spatial and energy domains.

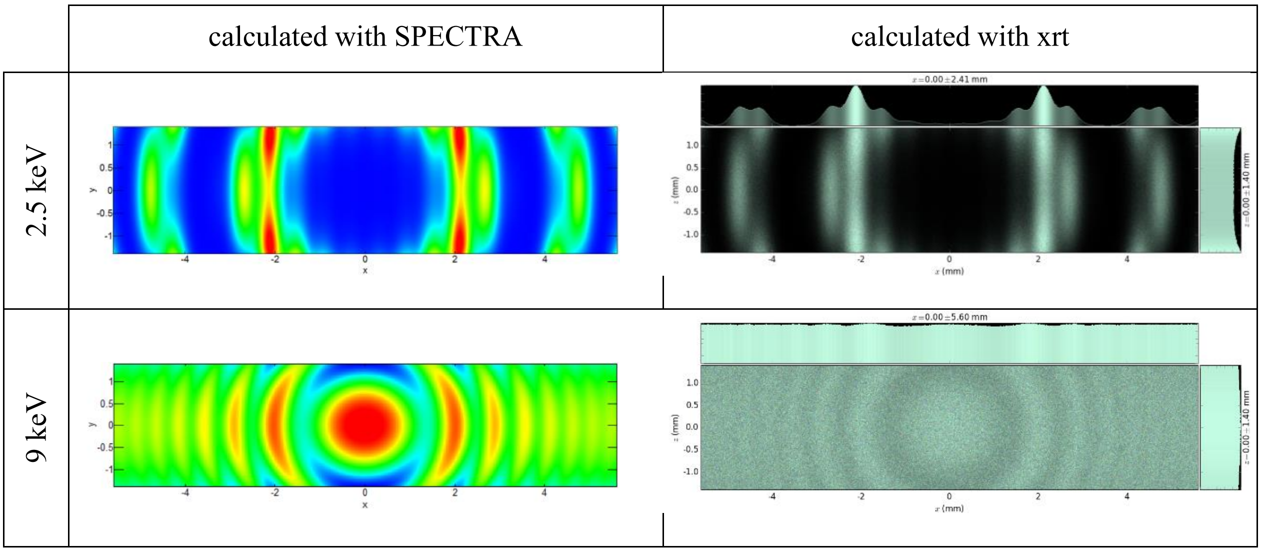

Figure 2. Beam cross-sections calculated with SPECTRA [3] and xrt [4] at two photon energies. SPECTRA represents intensity by color mapping; xrt represents intensity by brightness while colors represent energy. Xrt additionally shows two 1D positional histograms. Apart from these two different ways of representation, the results look very similar.

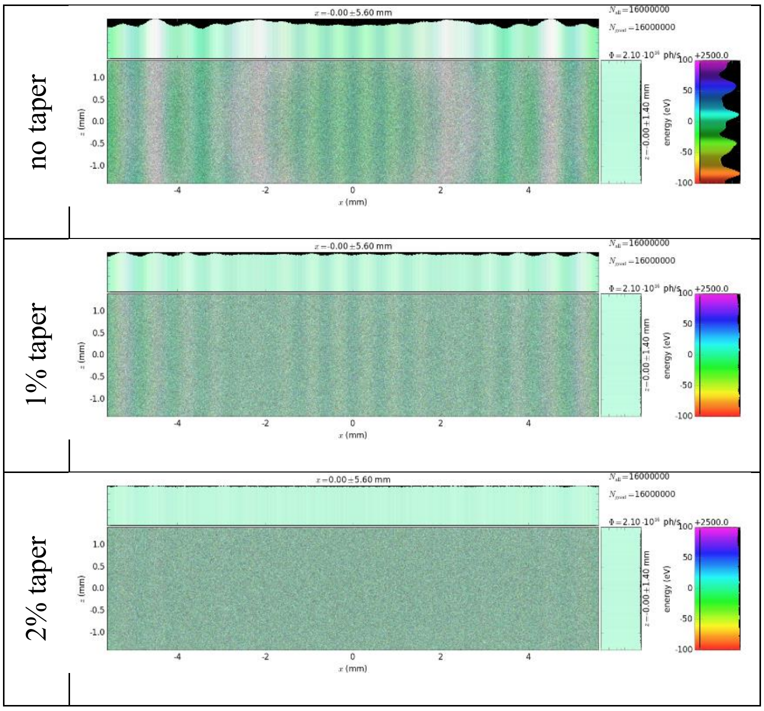

Figure 3. Beam cross-sections and energy distributions calculated with xrt at different gap tapering levels.

2.2. *The Optics*

The front end accepts 0.4h×0.1v mrad^2 of the wiggler radiation with up to 1.2 kW power in the beam. This power is distributed among three filters, a collimating mirror and the first crystal of a double crystal monochromator (DCM). The latter typically absorbs up to 500 W, in one particular regime – up to 750 W. Therefore, the monochromator is cryogenically cooled. The collimating mirror absorbs up to 800 W and is cooled via grooves filled with liquid metal.

The beam at the sample is focalized into a ~100h×100v μm^2 spot by a toroid mirror. There are two toroids with different coatings to serve different energy ranges. In order to minimize the realignment time, the two toroids have equal sagittal radii. The beam at the sample can be unfocused up to ~4.5h×2v mm^2 by going off the nominal 2 mrad pitch angle of the mirrors. In order to minimize the realignment time and simplify the end station, the height of the focusing mirror and all the downstream elements is kept invariant under changes of the mirror pitch angle. This can be achieved by a relatively long range of the fixed exit offset of the DCM within 10–32 mm. The DCM is foreseen to be operated in fixed exit mode, but with the possibility to be operated in pseudo channel-cut mode as well, for faster data acquisition time. The DCM has direct drive mechanism in order to operate the Bragg angle at a speed of up to 5^0/s. The transmitted flux onto the sample by the two DCM crystal pairs, Si 111 and Si 311, is 10^{12}–10^{13} ph/s as estimated by ray tracing using xrt [4] in various assumptions about optical quality of the mirrors.

3. The experimental station

The experimental station requires an easy exchange between different experimental set-ups for both transmission and fluorescence XAS measurements, as well as auxiliary instrumentation and sample preparation laboratory. It is required to have a variety of detectors for fluorescence measurements accessible to the users. An ongoing project is in-house development of an X-ray emission spectrometer, which will be used as the standard florescence detector, for performing site selective XAFS spectroscopy measurements and also as an X-ray Raman spectrometer for probing soft X-ray absorption edges. The spectrometer is also presented in this proceedings volume [5]. Additional detection system that will be available to the user community is a set of standard fluorescence detectors, ranging from Lytle and PIPS detectors to a four-element energy dispersive silicon drift detector. The silicon drift detector will be equipped with an Xpress 3 pulse processor that gives count rates of $3 \cdot 10^6$ counts/element.

Additional instrumentation available for user experiment is a closed cycle cryo-cooler that operates with exchange gas in the sample compartment for temperatures down to 4 K, and a gas delivery system, for pressures ranging from atmospheric pressure to up to 30 bar, equipped with a mass spectrometer. The experimental station is developed to incorporate auxiliary methods in such a way that techniques like Fourier transform infrared (FTIR) spectroscopy, UV-Raman spectroscopy, X-ray diffraction and/or mass spectrometry can be performed simultaneously as the XAS study. It will be a flexible system where different instruments can be plugged in and out depending on the needs for the particular investigation.

Acknowledgments

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References

[1] Marcouillié O. *et al*. 2010 *AIP Conf. Proc.* **1234** 556
[2] Welter E 2012 *J. Synchrotron Rad.* **19** 905
[3] Tanaka T and Kitamura H 2001 *J. Synchrotron Rad.* **8** 1221
[4] Klementiev K and Chernikov R 2014 *SPIE* Advances in Computational Methods for X-Ray Optics III, 92090A; doi:10.1117/12.2061400
[5] Klementiev K, Preda I, Carlson S, Sigfridsson K and Norén K 2015 *High performance emission spectrometer at Balder/MAX IV beamline*, this volume.