The Energy Materials in-Situ Laboratory Berlin (EMIL) at BESSY II

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The Energy Materials in-Situ Laboratory Berlin (EMIL) at BESSY II

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Abstract. The Helmholtz Center Berlin (HZB) and the Max-Planck Society (MPG) strengthen their research in renewable energies with the implementation of the joint Energy Material in-Situ Lab Berlin (EMIL) at the third generation light source BESSY II. The new facility is dedicated to the in-situ and in-system x-ray analysis of materials and devices for photovoltaic applications, (photo-) catalytic processes, energie conversion and storage. To obtain a comprehensive understanding of the involved materials, spectroscopic methods with x-rays from the soft- up to the hard x-ray regime reveal an almost complete picture of their chemical and electronic properties. The contribution presents the layout of the x-ray beamlines and their performance in terms of photon flux, energy resolution and spot sizes.

1. Introduction

The EMIL project combines the research activities of two major facilities, the HZB and the MPG, in a sustainable energy supply based on renewable energies. The end station named SISSY was designed for the investigation of photovoltaic devices and materials under *in-system* conditions of the fabrication process, whereas the CAT end station studies (photo-)catalytic materials and processes under ambient conditions with spectroscopic methods. Hot topics are the (photo-)catalytic dissociation of water, energy storage and the electrochemical processes in the formation of solar fuels. The large variety of available methods in the end stations (PES, PEEM, HAXPES, XES, XAS, XRF, XRD) enables the investigation of sample structures with information depths ranging from a few nanometers up to the micron scale. For the preparation of thin film photovoltaic devices, state of the art quasi-industrial deposition tools will be available on-site. Up to three deposition clusters for different material types are planned: a thin film poly-Si cluster, a cluster for Cu(In,Ga)(S,Se)$_2$-preparation and a cluster for completely new photovoltaic nano-materials. The production of fully functional test devices and corresponding witness samples will be possible. The witness samples will be directly transferred via an UHV-system to the x-ray analytics stations, so that samples as close as possible to the status nascendi can be investigated. The beamlines in this project must deliver x-rays from 70 eV up to 8 keV to the end stations SISSY and CAT. This is realized by the installation of two undulators for soft and hard x-rays, respectively. The beamline layout must allow for a parallel operation of both beamlines for either the CAT or the SISSY end station, as well as for a parallel operation of both end stations with either the hard x-rays or the soft x-rays, respectively. A similar setup with two undulators and a combination of hard and soft x-ray beamlines is currently commissioned at the Diamond Light Source (I06) and is planned at the Shanghai Synchrotron Radiation Facility.

2. Undulators

Two undulators are planned to deliver photons with energies from 70 eV to 8 keV. An elliptical APPLE II undulator with a period length of 48 mm, 31 periods and a maximum k-value of 3.4 will cover the soft x-ray regime from 70 eV to 2200 eV and a planar cryogenic in-vacuum undulator with a period length of 16.25 mm, 92 periods and a maximum k-value of 1.5 is foreseen for the hard x-ray regime up to 8 keV. The calculated values for the photon flux of both devices are shown in Figure 1. Both undulators are installed in the same low-β section of the BESSY II storage ring. The installation of two undulators with a chicane in-between necessitate a modification of the electron beam optics, which has already been tested and approved [1]. The cryogenic undulator with a minimum gap of only 5 mm and will be installed upstream of the soft x-ray undulator [2]. The angular separation of both undulator beams is determined by the opening angle of their emission cone. A minimum acceptance of 0.55 mrad is required for the soft x-ray undulator to accept 5 sigma of the coherent cone at the lowest photon energy and an acceptance of 0.45 mrad for the hard x-ray undulator, respectively. For a reasonable separation of the beams and some safety margin, a canting angle of 2 mrad between both devices has been selected.

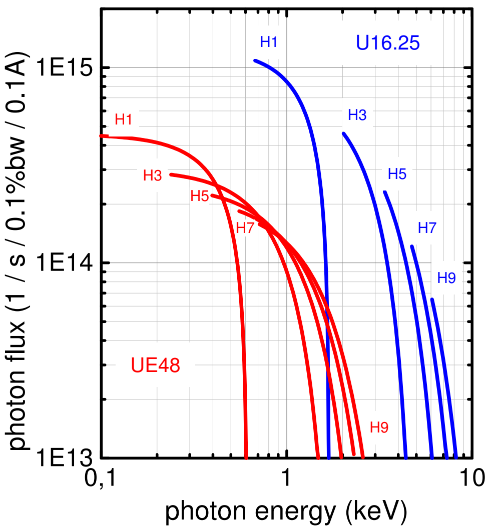


Figure 1. Photon flux of the two undulators. Red, the photon flux in the first, third, fifth and seventh harmonic of the low energy undulator, blue, the corresponding values for the high energy undulator.

3. Beamline

The schematic beamline layout of the EMIL facility is shown in Figure 2. Two independent beamlines, a hard x-ray beamline sketched in blue (dark) and a soft x-ray beamline sketched in red (light), are in close proximity. The components are shown schematically. Their positions (in meter) are given with respect to the center of the straight section in the storage ring. Numbers between components (green) indicate the lateral distance to the adjacent beam of the other beamline (in millimeter). The areas shaded in grey show the dimensions of the existing ring tunnel, the experimental floor, the walk around and the projected new EMIL building. Between the existing building and the new EMIL-Laboratory a small corridor, marked in white, has to be kept free for safety reasons. With the canting angle of 2 mrad, the two undulator beams propagate until their separation is large enough to mount two separate mirrors. These two mirrors are mounted within the ring tunnel at distances of 11 m and 13.5 m, respectively. This keeps the bremsstrahlung within the ring tunnel and eases the radiation safety measures in the experimental hall. After the first mirrors, the angular separation of the two beams increases to 1.2° allowing for the setup of two dedicated beamlines. The soft x-ray beamline is attached to the UE48 undulator and is based on a collimated plane grating monochromator with a grating chamber (GCs), a switching mirror unit (SMUs) and two branches with two exit slits. Two blazed gratings with line densities of 400 l/mm and 800 l/mm, respectively, and a blaze angle of 1° are foreseen. The variable deflection angle at the grating will be realized by means of a tilting mirror in the SX-700 geometry. The SMUs holds two face to face mounted mirrors for focusing to the branches for SISSY and a PEEM station. Switching is performed by a linear translation of the mirrors. When both mirrors are out of beam, the transmitted beam is focused by a stationary mirror to the CAT-branch. Refocusing optics in all branches transport the beams into the corresponding end stations. The hard x-ray beamline is attached to the planar U16.25 undulator. The toroidal first mirror deflects the beam for radiation safety reasons and collimates it vertically. Horizontally it will be focused to a distance of 36 m. It is then directed to a double crystal monochromator (DCM) with a silicon (111) crystal pair. Afterwards, the beam is focused by one of two mirrors in a switching mirror unit (SMUh) onto slits in two branches. The double crystal monochromator covers the energy range above 2 keV with the third harmonic of the U16.25 undulator.

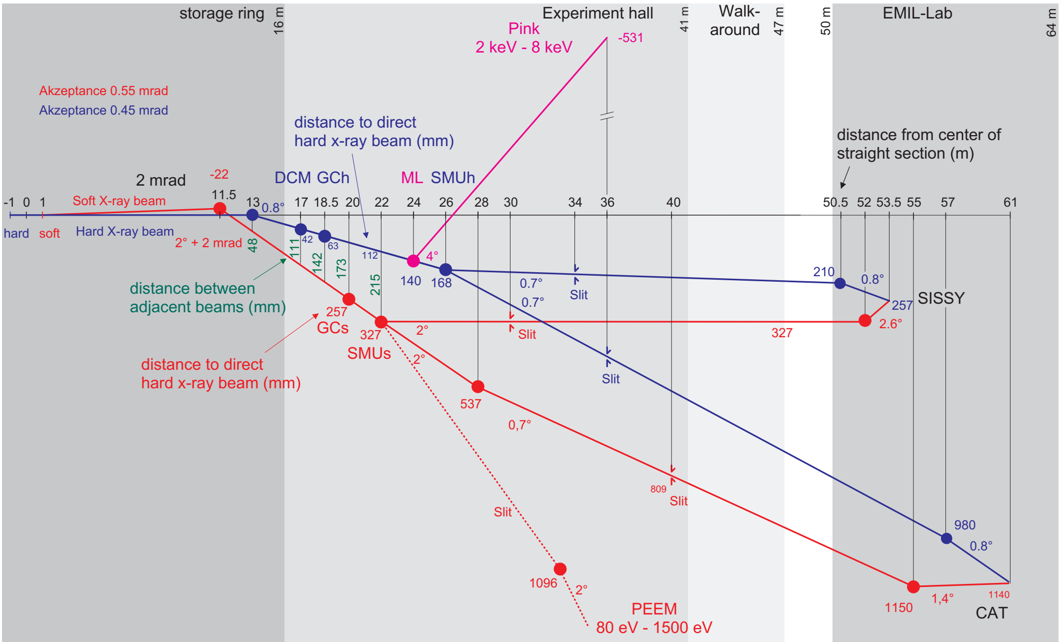


Figure 2. Schematical overview (top view) of all beamlines projected for EMIL. All beamlines and end stations stay essentially in the plane of the storage ring. A height offset of about 20 mm occures downstream of the grating chambers (GCh,GCs) and double crystal monochromators (DCM).

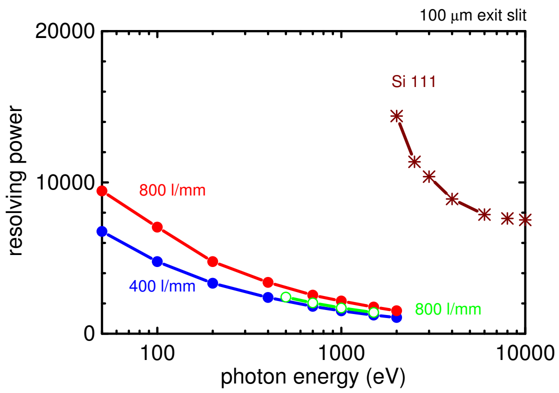
Unfortunately, the DCM cannot handle the first harmonic of this undulator, which carries a significantly higher photon flux compared to the UE48 in this spectral range. To exploit the first harmonic in the hard x-ray beamline, a grating chamber (GCh) will be installed behind the DCM. The DCM must then clear the beam path for the operation in the first undulator harmonic. This can easily be realized by a translation of one or both crystals sideways. With a similar translation of the grating in the GCh, the beam can pass this chamber when the DCM is operational. In both operation modes, the grating and the crystal act in collimated light. The subsequent focusing in the SMUh at 26 m and in the refocusing chambers is therefore unaffected. The exit slits are only effective when operating in the grating mode. In the crystal mode the slits are opened. The beams of the hard x-ray and the soft x-ray beamlines are overlapping in the SISSY and CAT end stations. Both end stations can operate with both beams available, or use either one or the other undulator, while the other end station uses the other simultaneously. The photoemission electron microscope (PEEM) exploits soft x-ray only, while the PINK end station uses only hard x-rays. The PINK-station has the option to use the direct undulator light. For that, the DCM and the GCh has to clear the beam path. A cylindrical mirror with up to six multilayers (ML) at 24 m distance, deflects the beam by 4°. The ML-mirror performs vertical focusing only, while the horizontal focusing is performed by the first mirror.

Table 1. Spot sizes (hor.× vert.) in µm at the end stations for 20 µm exit slit width.

	Soft x-ray		Hard x-ray		
End station	80 eV	1000 eV	700 eV	2000 eV	8000 eV
SISSY	35 × 3	33 × 2	170 × 20	120 × 8	120 × 5
CAT	180 × 25	120 × 10	160 × 25	120 × 8	125 × 6
PINK	-	-	-	570 × 25	570 × 20

4. Performance

The performance of the beamline was calculated with the code RAY. [3]. Photon flux and resolving power for the CAT end station are shown in Figure 3. The values for the SISSY end station are about the same. The solid dots show the performance of the soft x-ray beamline with grating line densities of 400 l/mm and 800 l/mm, respectively. The photon flux is calculated for gold coated elements with horizontally polarized light from the UE48 and an exit slit opening of 100 µm. Data points marked as stars show the performance of the DCM-beamline, starting at 2000 eV. A beryllium filter with 100 µm thickness blocks the undispersed light and is included in the calculation of the photon flux. The open dots correspond to the grating mode of the hard x-ray beamline operated with the UE16.25. The photon flux for a 800 l/mm grating is plotted with and without a beryllium filter to compare it directly to the values of the soft x-ray beamline or the DCM-mode. The spot sizes at the end of the branches are calculate for all end stations and are listed in Table 3. The values are calculated for an exit slit setting of 20 µm (soft x-ray beamline) and give the minimum achievable spot sizes on the samples, which are relevant for the design of secondary photon and electron spectrometers at the end stations.



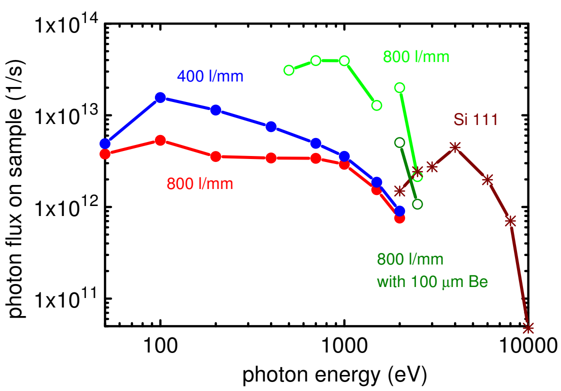


Figure 3. Photon flux and resolving power at the CAT end station for 100 µm exit slit width.

5. Outlook

The design of the beamlines with the number and positions of the end stations is now completed. The tendering process for the beamline is ready to start. The EMIL facility will become operational in 2015 and will open exciting possibilities for in-situ and in-system x-ray analysis of materials and devices for photovoltaic applications and of (photo-)catalytic processes under working conditions.

6. References

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