

Beamline Review Report

The Bloch beamline team

April 2022

This report has been compiled to facilitate the 2022 external review of the Bloch beamline at MAX IV. It aims to provide sufficient background to assist the review committee in answering the charge questions listed in Section 1.1.

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1 General introduction and charge questions

Bloch is a low-energy (10-250 eV) beamline on the 1.5 GeV electron storage ring at the MAX IV Laboratory, that has as its singular focus angle resolved photoemission spectroscopy (ARPES). There are two branchlines at Bloch serving two permanent endstations. The optical parameters are essentially identical between the two branches; the differentiation comes from the capabilities of the endstations.

The first endstation (A-branch) offers high resolution ARPES with a Scienta DA30L analyzer and a 6-axis cryomanipulator. Additional unique features of the endstation are a UHV coupled scanning tunneling microscope and two preparation chambers for evaporating material, gas dosing or annealing. The A-branch has been in general user operation since September 2019 (2.5 years).

The second endstation (B-branch) features a 3D VLEED detector combined with a Specs Phoibos 150 analyzer, making spin-resolved ARPES its defining feature. Furthermore, the endstation was designed to facilitate rapid exchange of the measurement manipulator, with the eventual aim of offering diverse sample environments for specialized experiments. This endstation is still in the commissioning phase and will open for general user operation in January 2023.

Bloch was designed with the flexibility to excel in several different technical aspects if given sufficient development resources. Since research with ARPES encompasses many different experiments which often have orthogonal requirements, this kind of flexibility was considered important for the beamline to remain relevant to a diverse user community. As it stands today, given the internal development efforts and the needs of the user community, the subset of features that have become the defining strengths of Bloch are:

- Small spot size
- Deflection analyzer
- High energy resolution
- Wide photon energy range
- Ease of operation

The importance of these properties will become apparent from the in-house and user science examples in Section 4.

Several aspects of the beamline have not yet been developed and exploited to their full potential - for example higher order suppression or the flexibility of the monochromator with respect to gratings and different cff settings. Since going into operation we have also identified new directions that were not obvious or even possible during the initial beamline design phase. These are discussed in Section 6.

We also wish to highlight the hybrid operation/commissioning status of Bloch at present. One endstation is in full user operation, a second is in the commissioning phase all while multiple large-scale development projects are being pursued concurrently. While development work will and should never stop, we can nonetheless expect that the focus and workload on the beamline staff will look quite different 3 years from now when both endstations are in stable operation mode.

Bloch was constructed with a budget of 75 MSEK (~ 7.2 M€). Today it operates on an annual running cost budget of ~ 350 kSEK (~ 35 k€), with the possibility to apply for internal funding grants of order ~ 200 kSEK (~ 20 k€) each for small upgrade projects. Staff salaries and travel expenses are covered separately.

In the next 3-5 years our aim is to be realizing more of the potential this beamline possesses, and to be widely known as a premier destination for both regular ARPES and spin-resolved ARPES.

1.1 Charge questions

Does the committee agree that the development projects for the coming years, as outlined in Section 6, represent the best allocation of our resources towards improving the beamline? Are there alternative directions that should be considered?

Is Bloch competitive today with similar facilities worldwide? Will we still be competitive in 5-10 years?

Is our current user community the size and composition it should be, considering the performance and age of the beamline? Are our outreach efforts sufficient?

Is the publication rate and impact of research at Bloch commensurate with the number of allocated proposals for a beamline of this performance and age?

Is the in-house program (encompassing both scientific and development/maintenance work) commensurate with the amount of beamtime allocated for it, considering the staff composition, roles and responsibilities?

2 Technical description

2.1 Beamline design

The optical design of the beamline was primarily performed by Rami Sankari, who is now at Tampere University (Finland) but was behind the design of several beamlines at MAX IV. For a more in-depth discussion about the decisions that went into the beamline design we refer the reader to his 'Detailed optical design report' provided as a separate document alongside this report, however we note that some aspects of the design have changed since that document was written in 2014. In the following sections we will discuss the elements of the beamline optics and present measurements illustrating its performance.

Bloch was designed with the principle aim of offering high resolution ARPES in the UV range (10-220 eV) with a very small spot size on the sample. Secondary goals included the ability to reach energies up to 1000 eV with limited flux (for core level spectroscopy), preservation of circular polarization at low energies and efficient higher order suppression.

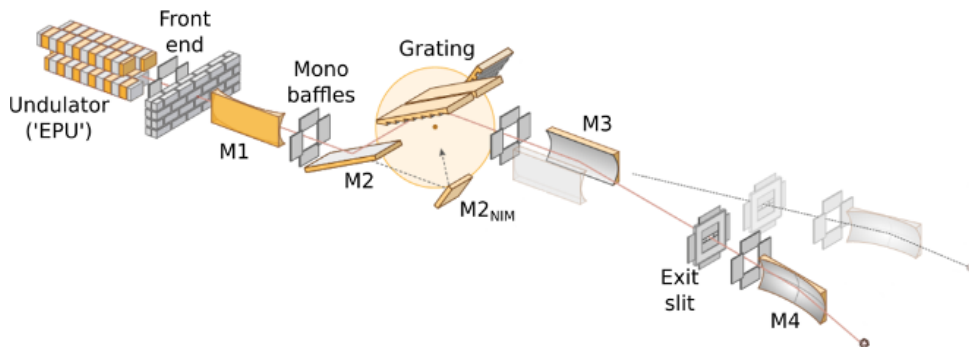


Figure 1: Overview of the beamline with all optical elements depicted

2.1.1 1.5 GeV ring and insertion device

While the 6 nm rad horizontal emittance of the 1.5 GeV storage ring at MAX IV cannot compete with the famously low emittance of the 3 GeV ring (200 pm rad), it is nonetheless competitive with state of the art third generation storage rings elsewhere in the world and provides an excellent foundation for a high-brightness UV beamline design. The beam size achieved in the center of the Bloch insertion device is $185\text{ }\mu\text{m}$ (H) \times $13\text{ }\mu\text{m}$ (V). Today it operates with a stored current of 400 mA and 30 minute top-up period.

Bloch is sourced by an in-house built quasi-periodic APPLE II type Elliptical Polarisation Undulator (EPU). The two primary targets setting the design were a fundamental harmonic that extended above 200 eV and high flux in the 10-1000 eV energy interval. The restrictions were a maximum length of 3 m and a minimum magnetic gap of 14 mm. The final design has 28 periods of vertical and horizontal pairs of glued permanent magnets. The period length is 84 mm and the minimum magnetic gap is 14 mm resulting in a lowest photon energy of 7.45 eV for horizontal linear polarization. A quasi-periodic magnet configuration was used to reduce higher order contamination, at the cost of a slightly reduced first harmonic intensity. This is achieved by shifting higher harmonics away from integer multiples of the first harmonic so that they will not make it through the monochromator. As shown in Figure 2, with the exception of the third harmonic in vertical polarization, this concept works well.

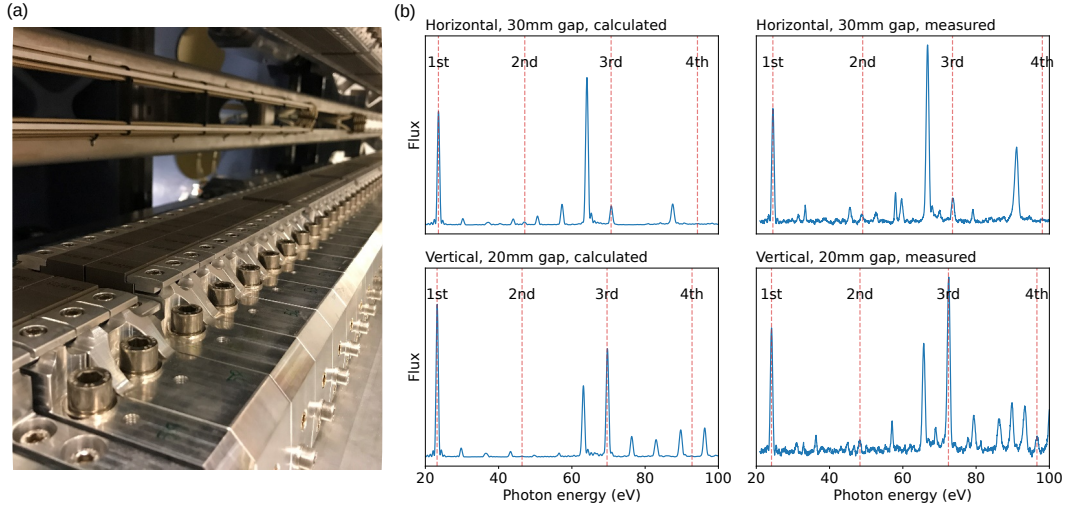


Figure 2: (a) Photograph of the Bloch undulator magnet lattice, illustrating the disrupted periodicity due to offset magnet blocks. (b) Calculated (left) and measured (right) undulator spectra for horizontally and vertically polarized light. The positions of the integer harmonics are highlighted.

2.1.2 Beamline optics

The first optical element of the beamline (M1) is a toroidal mirror, positioned 14 m after the source, that collimates the beam vertically and focuses it horizontally on to the exit slit. The large radius of the mirror deviates from design specification; as a result the incidence angle had to be changed from 3.0000° to 3.0114° which also meant that the horizontal focus moved about 1 m downstream as compared to the original optical design.

Bloch uses a collimated plane-grating monochromator (cPGM), placed two meters downstream of M1, which introduces a vertical beam offset of 42 mm. It can be reconfigured into a normal incidence monochromator (cNIM) mode. The standard configuration is cPGM mode with the 800 l/mm grating, but there are two additional cPGM gratings installed to afford flexibility in configuring the appropriate intensity vs. resolution tradeoff. Relative to the 800 l/mm configuration, the 2400 l/mm offers higher resolution while the 92 l/mm grating sacrifices resolution for intensity and is mainly intended for spin-resolved measurements on the second station. The 92 l/mm grating can also be used for better preservation of circular polarization. Technical specifications of the gratings are illustrated in Table 1.

The NIM mode was included in the monochromator design to preserve the photon beam polarization produced by the undulator at low photon energies and has its own grating and M2 mirror. This mode, as well as the 92 l/mm and 2400 l/mm cPGM gratings, have been installed and tested, but have not been thoroughly calibrated and are not yet in demand from users. It should be added that in the initial beamline design, before the quasi-periodic EPU was introduced, the NIM grating was also intended to be used for suppression of higher order light. Following the later decision to use a quasi-periodic undulator, this aspect is now of less importance.

Positioned 1 m after the monochromator, M3a and M3b are cylindrical mirrors that focus the beam vertically on to the exit slit of branch A and branch B, respectively. The swapping of the beam between the branches is accomplished by translating the respective mirror horizontally into the beam. The deflection angle at M3a/b was changed from 6.0000° (design specification) to 5.3111° due to the adjusted angle of M1, in order to still achieve a stigmatic focus at the exit slit.

The exit slits of both branchlines are positioned 10.166 m after the M3 mirrors. The size of both the horizontal and vertical exit slit openings can be controlled, as well as their longitudinal position along the beam. On the A-branch the exit slit mechanism is housed in a gas filter assembly in order to provide an additional means of filtering out higher-order light. The B-branch is prepared for this

option as a possible upgrade.

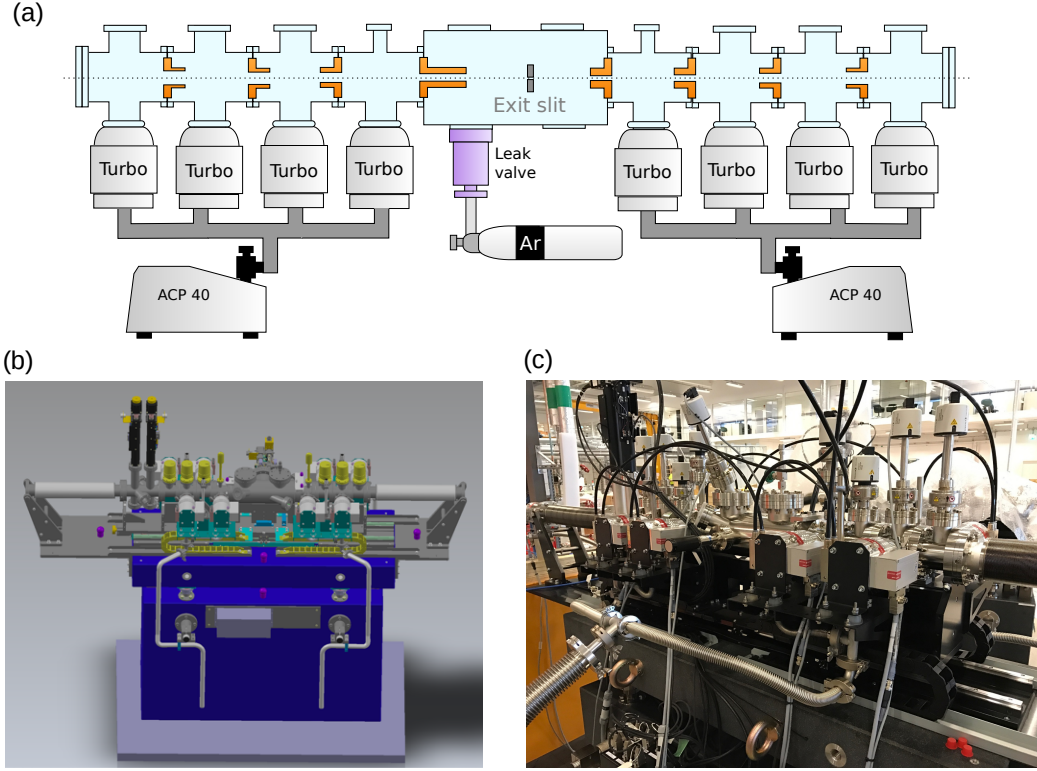


Figure 3: (a) Design of the gas filter exit slit assembly on the A-branch. (b) Final CAD model, and (c) photograph of the installed assembly.

The exit slit and gas filter unit on the A-branch is based on an in-house design, with construction contracted to Toyama. The unit can be filled with absorbing gases up to 3 mbar. The central exit slit chamber is differentially pumped by four turbo pumps mounted on either side on cells that are connected by ~ 2 mm diameter capillaries. The inner diameters of the capillaries are adjusted to account for the convergence and divergence of the photon beam before and after the exit slit. In addition, and not shown in Fig 3, there is another turbo pump and in-line ion pump on either side of the gas filter. With this setup, the gas filter does not disturb the upstream or downstream UHV conditions of the beamline, even when the central cell is operating at several mbar. There is also an ion pump on the central exit slit chamber for use when the gas filter is not in operation. The gas filter has been tested but not yet commissioned for general user operation.

The final optical element on each branchline is an ellipsoidal re-focusing mirror (M4a/b) positioned 10 m after the exit slit. It refocuses the diverging beam leaving the exit slit to the sample position, 1 m away in the analysis chamber. The refocusing is such that a ratio of 10:1 is achieved, i.e. an exit slit setting of $100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$ will be focused to $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m}$ at the sample position. A summary of the optical elements is given in Table 2.

2.1.3 Measured performance

Energy resolution The energy resolution of the beamline has been characterized by measuring photoionization (Rydberg) features in a gas cell containing 5×10^{-4} mbar of He ($2,1_3$ feature at

	Groove density (1/mm)	Optical size (mm)	Substrate	Coating	Tangential / sagittal slope error (arcsec)	Profile
PG1	2400	15 x 134	Silicon	Au	0.022 / 0.017	4.6° blazed
PG2	92	15 x 134	Silicon	Au	0.042 / 0.054	1.5° blazed
PG3	800	15 x 134	Silicon	Au	0.031 / 0.034	2.2° blazed
NIM	4000	20 x 20	Silicon	B ₄ C	0.013 / 0.018	Laminar, h=11, c/d=0.51

Table 1: Characteristics of the gratings installed at Bloch.

Optical element	M1	M2	M2NIM	M3a/b	M4a/b
Shape	toroid	plane	plane	cylindrical	ellipsoidal
Deflection	horiz.	vert.	vert.	horiz.	horiz.
Distance (m)	14	variable	16.053	17	37.163
Incidence angle (°)	3.0114	0-21	75	5.3111	3
Geom. size (mm)	360x40x60	620x60x60	70x40x60	220x80x40	240x80x65
Opt. size (mm)	340x20	550x15	20x20	200x600	200x60
Substrate	Si	Si	Si	Si	Fused silica
Coating	Au	Au	Au	Au	Au
Roughness (Å)	3	1.8	5	2.6	3.0
Slope error (arcsec)	0.15/0.8	0.039 / 0.056	0.050/0.062	0.1 / 0.25 ,	0.49/1.9
Entrance arm (m)	14	-	-	-/inf	10
Exit arm (m)	13.167 / inf	-	-	-/10.167	1

Table 2: Summary of mirror optics in the Bloch beamline. Slope errors are stated as (tangential slope error/sagittal slope error).

62.8 eV)) or Ne (16s'/15d' features at 21.5 eV). The measured resolution is consistent with predictions based on ray-tracing calculations. Figure 4a shows an overview spectrum of Neon using the 800 l/mm grating with $cff=6$. Figure 4b shows the resolution with the same grating as a function of exit slit opening, as determined by a fitting a box-convolved gaussian doublet to the feature highlighted in Figure 4a. In Figure 4c we show similar measurements for taken from a higher energy feature in He, this time comparing the 800 l/mm and 2400 l/mm grating at $cff=2.25$. The flattening of the energy resolution at small slit width is due to the diffraction limited source size and is reproduced by ray tracing simulations. This is essentially implying that the beamline energy resolution is primarily source size limited at least up to 60 eV). Ultimately the most important parameter for the users is the final energy resolution of photoemission from a sample. This is typically determined by fitting to the Fermi edge of a cold polycrystalline Au film, as shown in Figure 4d. The final experimental resolution is a convolution of the electron analyzer and the beamline contributions, and in real experiments is often dominated by the analyzer. While the analyzer was shown to be capable of 1.9 meV energy resolution in factory acceptance tests, in the real installation grounding issues and electrical noise can dramatically degrade this. The value of 3.2 meV shown in Figure 4d is the best we have obtained to date. More typically we can offer users an ultimate resolution of 4-5 meV, but without constant vigilance it is easy for seemingly trivial alterations or errors in the electrical cabling of the measurement chamber to degrade this to 20 meV or higher.

Flux The beamline flux has been characterized for all modes of operation using a silicon diode (IRD XUV100G) placed after the final M4 mirror. Figure 5a gives an overview of the flux and working range for each mode. Note that here the curves correspond to a fixed $cff=2.25$ and a fixed exit slit

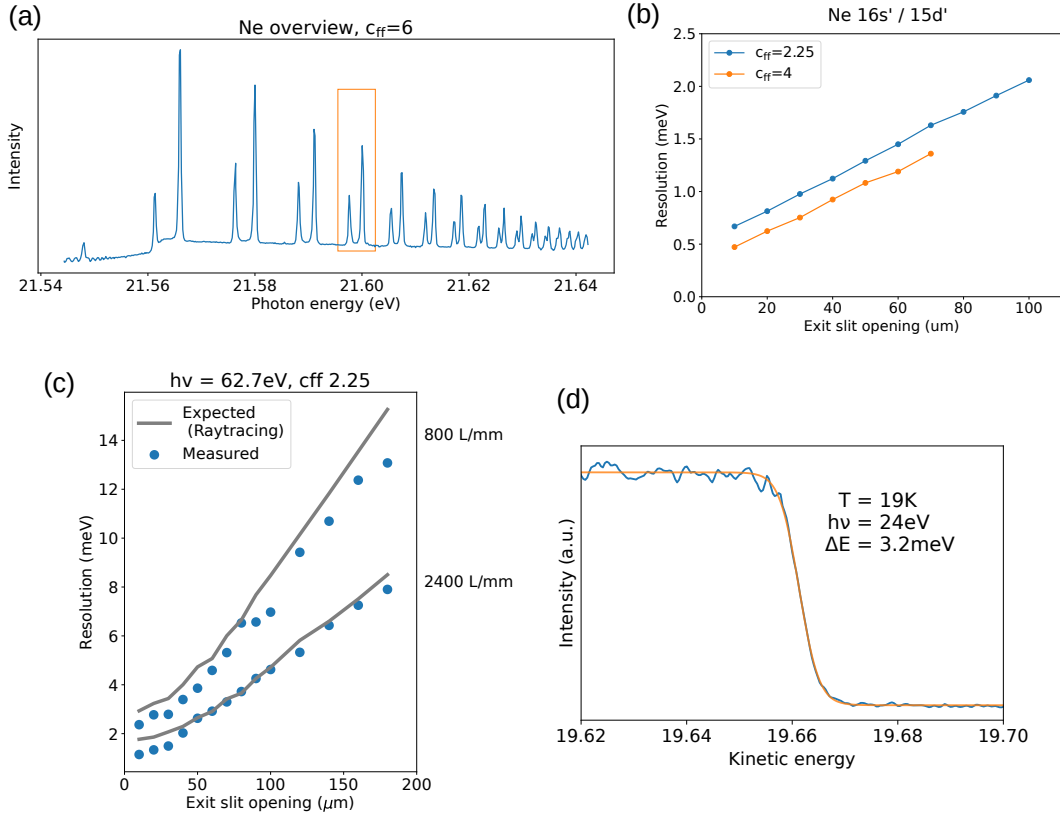


Figure 4: Energy resolution measurements. (a) High resolution ionization spectrum of the 16s'/15d' feature using a Neon gas cell and the 800 l/mm grating. (b) Exit slit dependent resolution of the doublet highlighted in (a), for the 800 l/mm grating at two different c_{ff} values. (c) Similar measurements for a higher energy feature in Helium, now comparing the 800 l/mm and 2400 l/mm gratings and including ray tracing calculations. (d) Ultimate energy resolution from the electron analyzer on a solid-state sample, with the beamline configured such that its contribution is negligible.

size ($100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$) that gives the minimum spot size, since this is typically the most relevant setup for users. The flux here is not the commonly quoted *flux at 0.1% bandwidth*, and so does not allow an easy comparison with other facilities. We are aware of the value of making values available in standardized form, and do plan to eventually collect this information during the next commissioning opportunity. Below 200 eV, all curves follow the first harmonic of the undulator. Above this value the undulator gap is closed to a fixed value of 20 mm and its broadband *wiggler* output is used. The inset plot (Figure 5b) shows good agreement between the measured and calculated flux for the 800 l/mm grating. Users appreciate the convenience of being able to use the entire photon range available without being forced to change gratings, and the flux is very often high enough that the exit slits must be closed beyond the resolution needs of the experiment solely to prevent damage to the detector. It is clear from Figure 5a that Bloch is not suitable for soft X-ray ARPES above 220 eV. Since photons with higher energy than this are considered a bonus and intended only for core level spectroscopy, the comparatively poor flux and energy resolution is not an issue.

Spot size The refocusing method at Bloch is based on a single ellipsoidal mirror that directly images and demagnifies the beam at the exit slit to the sample position. A consequence of this is that baffling the beam at the exit slit is reflected as a decreased image size. In the vertical direction this comes

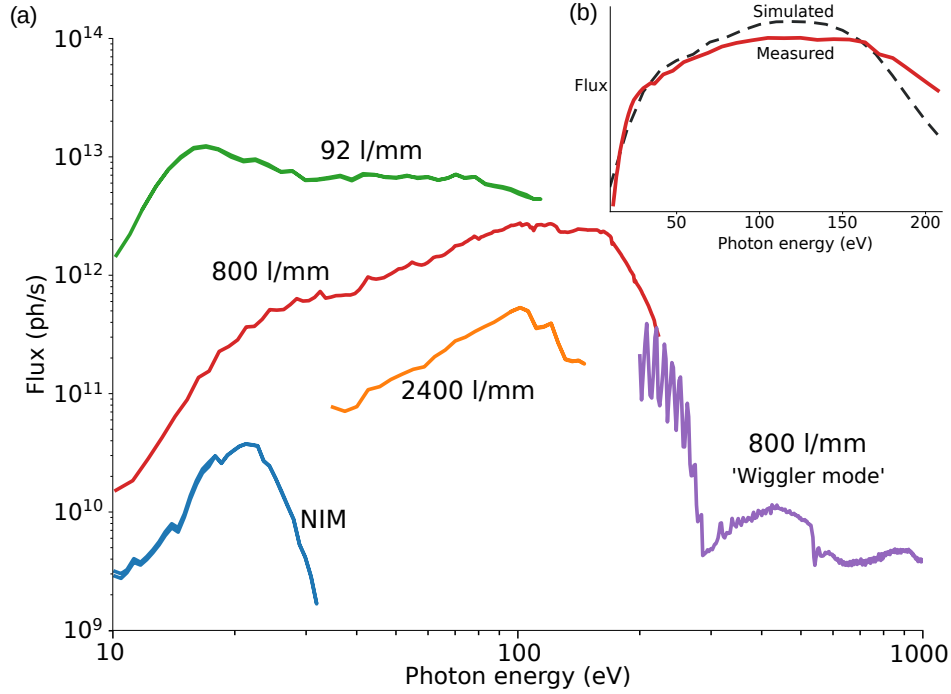


Figure 5: (a) Photon flux for all modes of operation at the beamline, measured with fixed exit slits and scaled to the intended final stored current of 500 mA (400 mA today). Exit slits were fixed at ($100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$) for all but the high energy wiggler mode ($50\text{ }\mu\text{m} \times 500\text{ }\mu\text{m}$). For all cPGM measurements cff was 2.25. Inset plot (b) compares the measured 800 l/mm flux with the anticipated curve based on ray-tracing calculations

naturally when closing the exit slit to improve energy resolution. The inclusion of a horizontal exit slit allows reducing the horizontal spot size by truncating the beam. In this way the minimum spot size of $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m}$ can be achieved by reducing the exit slits to $100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$; for these settings the flux and resolution of the beamline remain excellent. For cases where spot size is less critical, the flux can be improved by opening the horizontal exit slit up to $800\text{ }\mu\text{m}$. Closing the exit slits to openings smaller than $100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$ does not reduce the spot size any further, as the limiting factor then becomes the slope error of M4. Note that since most samples are measured closer to normal emission than normal incidence, the horizontal footprint of the beam on the sample is typically enlarged by $\sim 30\%$.

The spot size at the sample position has been verified using a test sample containing lithographically patterned Au on a Si substrate (Figure 6a). By tuning the spectrometer to a feature unique to Au (e.g. Au 4f core level at higher energies or metallic Fermi edge at low energies) and scanning the sample across the beam, the resulting spectrum reflects the lithographic pattern convolved with the photon spot size. The manipulator motion can be calibrated by measuring two features with a known separation. Figure 6b shows a 2D map performed in this way, while high resolution 1D scans across $5\text{ }\mu\text{m}$ Au lines are shown in Figure 6c. In this case, the spot size for 200 eV photons with $100\text{ }\mu\text{m} \times 100\text{ }\mu\text{m}$ exit slits yields a spot size ($h \times v$) on the sample of $7.7\text{ }\mu\text{m} \times 14.9\text{ }\mu\text{m}$, which maps to a beam size at normal incidence of $7.7\text{ }\mu\text{m} \times 9.6\text{ }\mu\text{m}$.

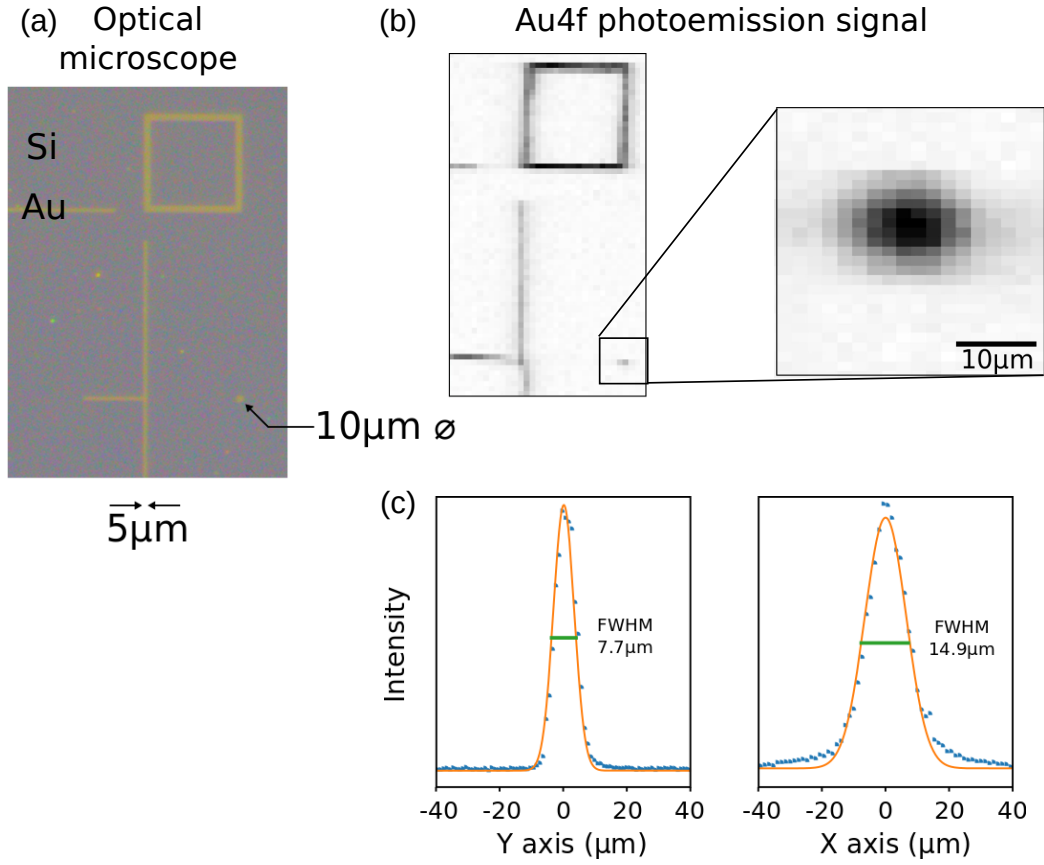


Figure 6: Characterization of the spot size on the sample. (a) An optical microscope image showing a section of the Au/Si test sample. (b) The same region measured by raster scanning the manipulator in front of the beam ($h\nu=200\text{ eV}$), with contrast generated by the magnitude of the Au 4f core level, together with a high resolution scan over a $10\mu\text{m}$ diameter circle feature. (c) 1D line scans over horizontal and vertical $5\mu\text{m}$ wide Au lines. The reported full width of the peaks is without performing any deconvolution.

2.2 The A-branch endstation: ARPES

2.2.1 Overview

The original planning for Bloch only included one endstation, the A-branch endstation, that was therefore designed with the flexibility to facilitate as wide a variety of user experiments as possible. This led to a design incorporating 7 coupled ultra-high vacuum chambers and has produced a highly successful endstation. Three main factors have led to this success: (i) the heavy time investment and eye for details of the beamline spokesperson Roger Uhrberg (Linköping University, SE) when supporting the Bloch team during the design and procurement phase; (ii) the valuable experience gained from running the two predecessor beamlines i3 and i4 on the MAX-III ring of the MAX-Lab facility and (iii) the heavy and continuous time investment from the Bloch team towards maintenance, upgrades and calibrations. The overall layout of the endstation is shown in Figure 7. In the following sections we describe each sub-system in detail.

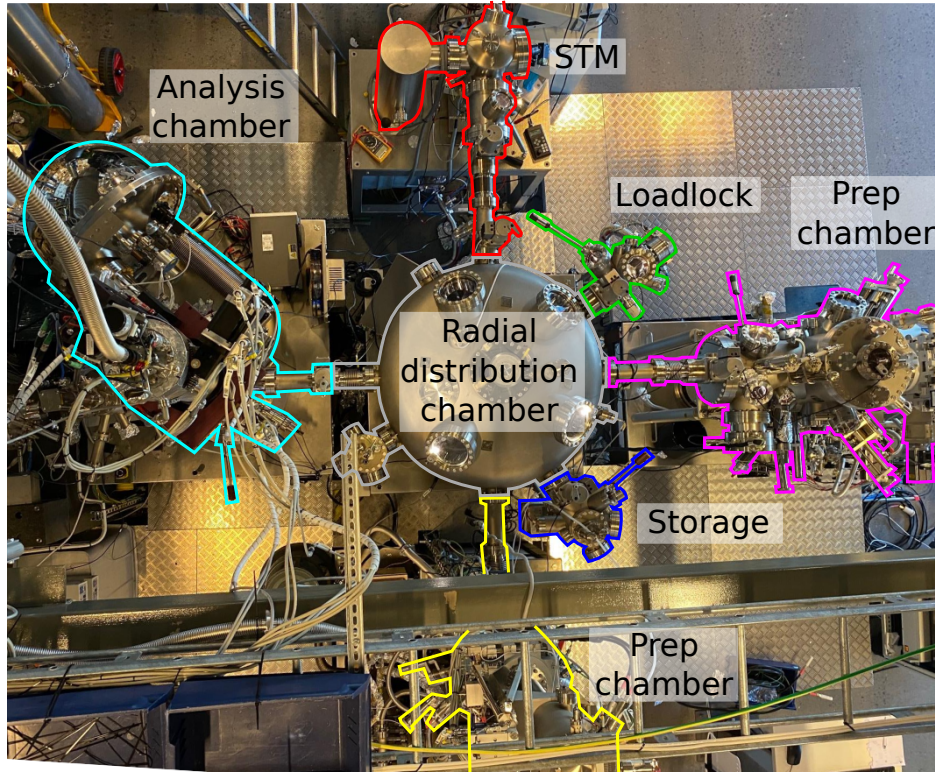


Figure 7: A-branch endstation layout illustrating all the UHV chambers. The photon beam enters from the left in this image.

2.2.2 Analysis chamber

The heart of the system is the Analysis chamber, equipped with a DA30-L hemispherical analyzer from Scienta-Omicron and a 6-axis Carving cryomanipulator from Specs. The chamber made of stainless steel with a double layer μ -metal lining. The measurement geometry is indicated in Figure 8; the manipulator hangs vertically, with tilt and azimuth as in-vacuum motions and polar derived from the differentially pumped rotational feedthrough.

The DA30L performs well and is well matched to the working range of the beamline. However, the ultimate energy resolution of 1.8 meV is not in practice achieved due to a combination of residual

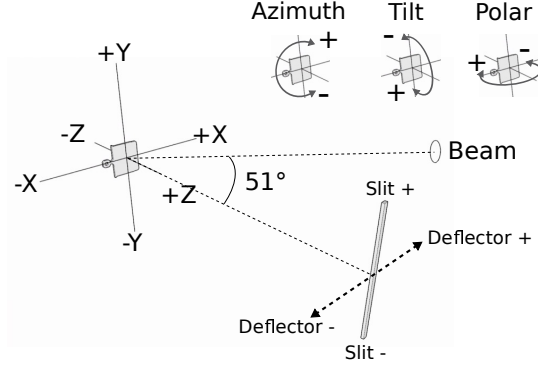


Figure 8: Measurement geometry

grounding issues (adding ~ 3 meV) and being forced to use higher pass energies (5–20 eV) at the kinetic energies we typically work with. Despite this, total energy resolution better than 10 meV is routinely achieved and when needed can be pushed below 5 meV. The electronic deflection capability - simulating a polar rotation without moving the manipulator - has been completely pivotal to the performance of the beamline. The small spot size attracts users with samples that are extremely small or non-uniform, and in such cases measurements that involve scanning a manipulator angle are infeasible. We have also seen that acquiring fast (< 2 min) deflector ARPES maps enables fast and precise sample alignment, and this feature is heavily used. One drawback of the DA30-L is the requirement of a field-termination mesh on the hemisphere exit, which generates artifacts in fixed-mode/snapshot ARPES measurements.

Despite having a deflection analyzer, the full 6-axis motion of the Carving manipulator is extremely important for precise sample alignment. While some motions present problematic backlash and cross-coupling of axes, overall the motion is stable and well behaved. The precision of the linear (1 μm) and angular (0.1°) motion is better than required, and the design of the Carving is such that there is relatively little motion of the sample when changing temperature. The range of motion has been sufficient for most experiments (see Table 3). The designed center of rotation is located 2.5 mm above the surface of the sample plate, corresponding to the surface of a wafer being held by a direct-heating style sample plate (cf. Fig. 9). Since measurements with scanned manipulator angles are relatively uncommon in practice, center of rotation issues are mainly only a consideration for making the angular alignment process simpler.

Bloch began operation using a liquid helium flow cryostat (supplied by default in the Carving, from manufacturer VAb) with a typical consumption in excess of 150 L for a 5-day beamtime to maintain a sample temperature of 21 K. In the beginning of 2021 we transitioned to low vibration closed cycle cryostats (Stinger from Coldedge) for the measurement chambers on both endstations. This has resulted in a slightly lower base temperature, has not coupled in any detectable level of vibration at the sample position and has greatly simplified the logistics and expense of coordinating LHe supply. The base temperature achievable at the sample is 19 K, which does not compare favorably to most other similar facilities where 10–15 K can be expected. In Section 5 we discuss this point in more detail, but we believe that one of the principle causes of this is inadequate thermal coupling between the sample and the receiver. sample clamping. Part of this stems from an unusual design requirement we made for the manipulator: at a specific azimuthal angle two electrical contacts are made to the sample that allow an electrical current of up to 10 A to be passed through the sample. This is a legacy feature from the design of the i4 endstation of MAX-Lab, where it was often used to flash-anneal samples without needing to transfer to a preparation chamber. In practice this feature has very rarely been used, although a small number of proposals have attempted to capitalize on it

in a different manner, for studying current-driven phase transitions.

Axis/Feature	Range/Value	Precision
x axis	no restriction*	1 μm
y axis	no restriction*	1 μm
z axis	no restriction*	1 μm
Polar	$-80^\circ \rightarrow +18^\circ$	0.1 $^\circ$
Azimuth	$-38^\circ \rightarrow +230^\circ$	0.1 $^\circ$
Tilt	$-25^\circ \rightarrow +30^\circ$	0.1 $^\circ$
Minimum temperature	19 K	0.5 K
Maximum temperature	420 K (150 $^\circ\text{C}$)	0.5 K

Table 3: Movement restrictions and precision of the 6-axis manipulator and temperature parameters.

* Enables access to all points on the sample plate.

2.2.3 Transfer system and sample holders

The endstation is configured to accept Omicron-style flag sample holders, both the flat plate variety and one that allows direct-current heating through a clamped sample (see Figure 9). Approximately half of the user groups bring their own plates, while the other half take from a stock of plates that we provide. A semi-automated radial distribution chamber (RDC) transfers up to two samples at a time between any two chambers, with transfer between manipulators exclusively performed manually with wobblesticks.

It is possible to cool with liquid nitrogen the RDC manipulator head below 100 K, enabling cold transfers between preparation and measurement chambers. While this is a useful feature to have and facilitates more exotic sample preparations, to date this has only ever been used for cleaving or depositing alkali metals on a sample while cold. Since both operations can now be performed on the measurement manipulator, the cold transfer option is almost never used.

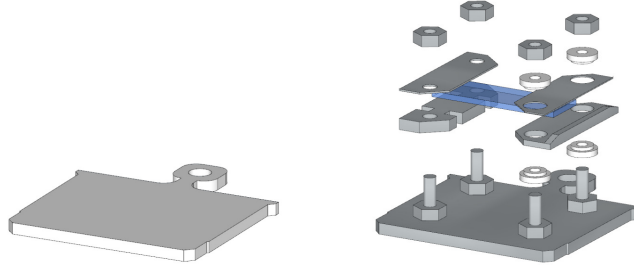


Figure 9: Flat and direct-heating style sample carrier plates used at Bloch, following the standard Omicron design

2.2.4 Sample preparation

There are two UHV preparation chambers for sample treatment and/or growth. The original design intent was to separate low- and high-vapor pressure processes, but in practice the main benefits have simply been redundancy and the efficiency of parallel operation. Both chambers have a 4-axis manipulator, LEED optics, thickness monitors and free ports with valves for mounting sources without venting the chambers. Cryogenic sample cooling is possible, although very rarely used. Heating is

possible with either resistive heating from a filament behind the sample receiver (max. 900°C), electron-beam heating of only the sample plate (max. 1400°C) or direct current heating by using the sample itself as a resistive element for currents of up to 12 A (>1200°C), as illustrated in Fig. 10. The flexibility of choosing the most appropriate heating style for the application at hand has proved to be valuable for enabling a wide range of sample preparations.

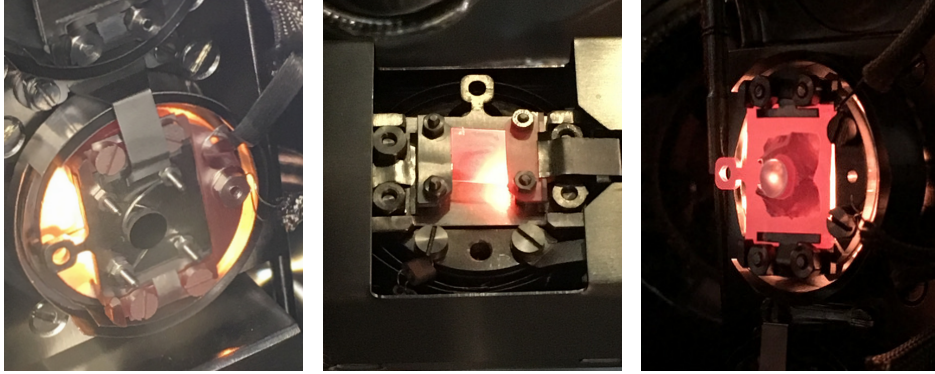


Figure 10: Resistive, direct and e-beam heating

With that said, for our user community at present, *in-situ* cleaving of top-posted single crystal samples is the most common preparation technique by a significant margin. When the beamline first went into user operation we did not permit cleaving in the measurement chamber based on concerns about where the top-posts would end up and on advice from Specs about the forces the Carving could handle. Eventually, however, we conceded to the overwhelming demand from the user community and developed a solution for cleaving on the Carving. Today this involves trying to catch the top posts in a small transferable basket, but a solution is being developed to transition to a simpler and more conventional ash-tray approach. For samples that require a lot of force to cleave or should be cleaved at room temperature, a dedicated robust cleaving receiver is available in a preparation chamber. Scotch-tape cleaving is typically performed in the loadlock.

2.2.5 Sample loading and storage

The loadlock has a 6-sample carousel and can be pumped to a suitable vacuum for transfer into the endstation ($<5 \times 10^{-7}$ mbar) within 2 hours. Resistive and direct-current heating is possible in the loadlock carousel for preliminary degassing. A dedicated UHV storage chamber offers a 12-slot carousel, while a further 12 slots are available in the STM chamber, if required. In practice the introduction of samples to the system is never a bottleneck during user beamtimes. Docking of vacuum suitcases to the loadlock or directly to a UHV preparation chamber is possible and has been used successfully.

2.2.6 Scanning tunneling microscope

An Omicron VT-XA scanning tunneling microscope is UHV coupled to the endstation, and is available to users either during their beamtime or, subject to scheduling and staff availability if required, before/after their beamtime. The instrument is routinely capable of atomic resolution imaging, even when the adjacent preparation or ARPES chambers are in use. In the right circumstances STM can offer a powerful complement to an ARPES experiment: providing real-space lattice measurements, identifying when multiple domains are contributing to the photoemission spectra and verifying a difficult sample preparation when LEED/ARPES are not sufficient. This is particularly true when it is possible to study the exact same surface that was measured with photoemission. The maximum frame size when imaging is $12 \mu\text{m} \times 12 \mu\text{m}$, while the coarse positioning range of $10 \text{ mm} \times 10 \text{ mm}$

permits access to all points on the sample plate. So far the STM has seen very limited use from the user community, but is extensively used to support in-house research. It has recently been upgraded to provide electrical contacts for measurements such as scanning tunneling potentiometry, and there is an ongoing in-house program to develop spin-resolved imaging.

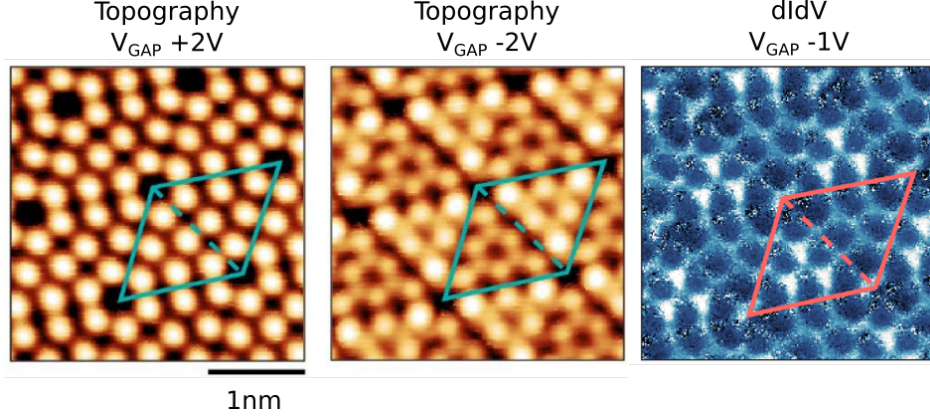


Figure 11: Example of atomic resolution topographic and dIdV imaging of a Si(111) 7×7 reconstructed surface.

2.3 The B-branch endstation: SARPES

2.4 Overview

The second endstation, on the B-branch of Bloch, is dedicated to spin and angle resolved photoemission spectroscopy (SARPES). It is installed and currently being commissioned, with the first officially approved expert commissioning beamtime scheduled for the second week of June 2022. While the flagship feature of this station is spin resolved photoemission, it was also designed to more easily accommodate manipulator exchanges and thereby enable customized sample environments.

The overall layout of the SARPES endstation resembles a slightly simplified version of the neighbouring ARPES endstation. It is built around an RDC for transferring samples between the different chambers, and features a single preparation chamber, a sample storage chamber and a load lock. The RDC has empty CF63 ports that can be used to dock new or temporary preparation chambers. In addition, a small preparation chamber is positioned on top of the analysis chamber. Here it is possible to perform simple sample preparations directly on the (vertically hanging) measurement manipulator, but the principle purpose is to act as a load-lock for the manipulator, enabling relatively rapid manipulator exchanges.

The analysis chamber is solid μ -metal for magnetic screening. We opted for a μ -metal chamber instead of a steel chamber with single or double μ -metal liners out of vacuum considerations. The chamber has a large top flange (200 mm diameter) to the preparation chamber above it to accommodate large sample stages on the manipulator. It is equipped with a Phoibos 150 SAL hemispherical electron spectrometer from Specs, mounted with the slit vertical and 45° to the incoming beam. The analyzer is equipped with a 3D VLEED spin detector (Ferrum + Specs) for spin resolved measurements. Also in the analysis chamber, facing the beam, we have a retractable polarimeter installed for characterizing the polarization state of the light at the sample position. It has very recently been installed and is currently entering the commissioning stage.

As mentioned, the small preparation chamber atop the measurement chamber permits users to install sample preparation or diagnostic tools or even exchange the entire manipulator, without needing to vent the analysis chamber and incur a 1-week turnaround time. This layout does impose the requirement of a very long manipulator travel length. A LEED unit for surface analysis or sample

orientation is permanently installed in this chamber, as are as wobble sticks for sample transfer and on-manipulator cleaving. The chamber is prepared for a retractable "waste basket" for simplifying the latter.

Once commissioned we believe that the existing sample preparation possibilities, storage chambers, an abundance of available ports - both on chambers and the radial distribution chamber, in combination with specific user supplied equipment will provide a flexible environment for the user community.

2.4.1 Analyzer and spin detector

The photoelectron analyzer on the SARPES station is a Phoibos 150 SAL from SPECS. This is a 150 mm mean radius hemispherical analyzer for angle resolved photoemission spectroscopy (ARPES), and features a scanning angular lens (SAL) ability analogous to the deflection capabilities of the neighbouring DA30-L analyzer. We anticipate that this functionality will again be invaluable, greatly simplifying the selection of k-points to measure. During site acceptance tests severe issues were seen with the quality of the slits. A replacement analyzer has been prepared and is scheduled for installation in May 2022.

The detection system after the hemisphere is a multichannel plate (MCP) detector read out by a CCD camera. Importantly, here it is also possible to electrostatically deflect the electrons past the MCP and through a series of transfer lenses into a VLEED spin detector. Due to the inclusion of a spin-rotator component it is possible to access full 3D spin vector information with a single VLEED detector. This is illustrated in Figure 12 - essentially the spin rotator enables disentangling the two in-plane vectors. Compared to the 2-VLEED solution offered by Scienta-Omicron, this approach has the advantage of using a single fixed target and detector, avoiding potential issues with beam alignment and normalization and simplifying operation and maintenance. Pragmatically, cost was a major factor in selecting this 3D-VLEED configuration over other multi-VLEED offerings. Since the spin endstation was not formally included in the initial beamline project funding, we faced more severe budget constraints when procuring it.

2.4.2 Manipulator

A 4-axis Omniax manipulator is presently used for the analysis chamber, i. e. with no in-vacuum angular motion mechanics. A project for upgrading to a 6-axis manipulator is on-going (see Section 6.3.2 for details). The same model of closed-cycle He cryostat from Coldedge (Stinger) is also used here for sample cooling. With the present sample receiver design, which does not include cryoshielding, the base sample temperature is 15 K.

2.4.3 Endstation status and commissioning plans

The SARPES station including all its sub-systems and components is currently being commissioned. The first external commissioning user group (selected by the Program Advisory Committee - PAC) is scheduled for June of 2022. A second call for commissioning users for the fall of 2022 was published earlier this year and three user proposals will be selected. There are still several steps to be taken before we can move out of the commissioning phase and into user operation, currently scheduled for spring of 2023. Some of these steps are summarized below.

- **Analyser** Due to a very high incidence of defects on the entrance slits it was decided in 2020 that SPECS would replace the present analyzer with a new one. This was considerably delayed due to the COVID-19 pandemic but is now ready and scheduled for installation in May this year. This will cause an interruption of approximately two weeks for installation work and tests. We believe that this will not interfere with the scheduled commissioning user beamtime in June.
- **Manipulator upgrade** A four-axis manipulator will be quite limiting in terms of what experiments are possible. See Section 6.3.2 for discussion about the upgrade project.

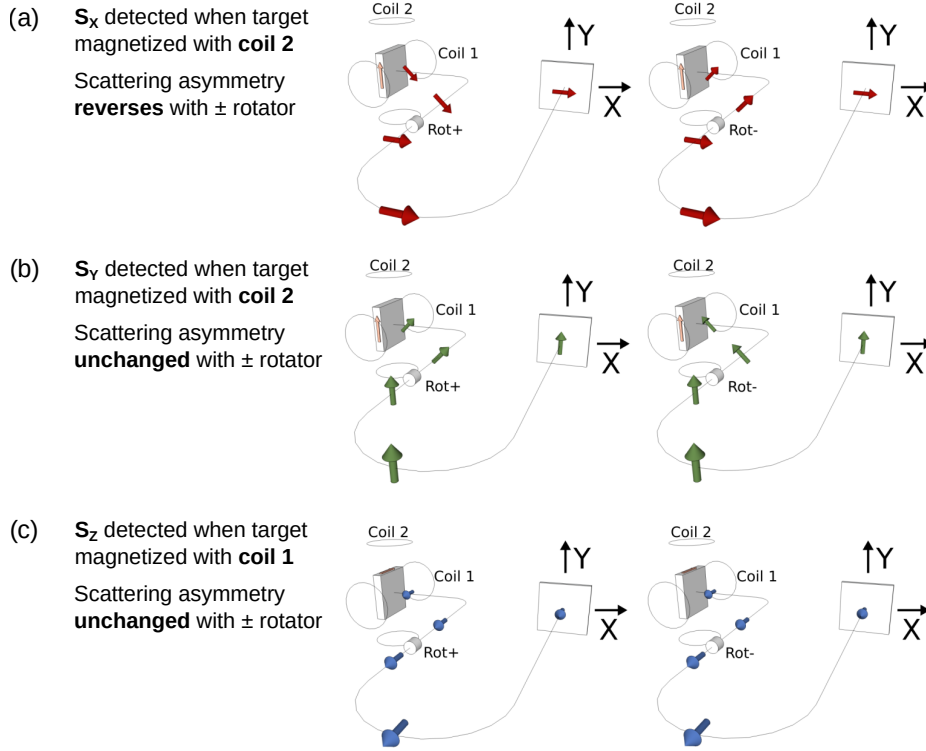


Figure 12: Illustration of the principle of 3D spin vector measurement with a single VLEED+spin rotator package. In this geometry the two in-plane components register together when the target is magnetized with coil 2, but can be disentangled by measuring with two different spin rotation operations. The spin rotator is a magnetic element located after energy and angle filtering in the hemisphere but before entering the spin detector.

- **Spin detector** Initial tests of the spin detector have been performed and were promising. We have confirmed that the detector can resolve spin states but more commissioning work is needed to verify the resolution (angle and energy) and reliability of the spin measurements. These tests will continue after the analyser replacement in May this year.
- **Polarimeter** A compact polarimeter has recently been installed in the analysis chamber and is currently being tested for basic motion. Time will be allocated for full commissioning. Its main purpose is to serve as a diagnostic tool to characterise the polarisation of the photon beam impinging on the sample. It will also be used within a larger project aimed at mapping out gap and phase settings for the EPU to provide fully controlled linear, inclined and circular polarized light at the sample position. The commissioning will be performed in parallel with the commissioning of the analyzer and spin detector, planned within the in-house beamtime allocated to Bloch. For more details, see Section 6.3.1.
- **Preparation Chamber** The large preparation chamber is being commissioned (in regard to motion, heating, sputtering etc.) and is close to being fully operational.
- **Software** The proprietary software (*Prodigy*) for the analyzer and spin detector is not as user friendly as we would like for a user facility, and we expect that it will need to be wrapped with an alternative user interface. This will mainly be developed by and at Bloch in collaboration with the MAX IV IT group (KITS). Control software for the polarimeter has been developed

by KITS, and the analysis routines will be developed at Bloch.

Where beam is required to complete these plans, time will be allocated from available pool of in-house time dedicated to commissioning, upgrades, maintenance and research across both endstations.

2.5 Bloch in context

2.5.1 Other ARPES possibilities at MAX IV

At MAX IV there are four VUV beamlines, all installed at the 1.5 GeV ring, where it is possible to perform ARPES measurements in some shape or form. These are Bloch, FinEstBeAMS, FlexPES and MAXPEEM. However of this group, Bloch is the only beamline designed for and fully dedicated to ARPES, and will be the only option for SARPES studies.

FinEstBeAMS is a multi-purpose EPU beamline. It has two branch lines, one of which has an endstation dedicated to XPS measurements of solid state samples. Here it is also possible to perform ARPES. The solid state endstation hosts a 150 mm Specs PHOIBOS analyser without deflectors. The manipulator has 5 axes and can be liquid nitrogen cooled. The analyser entrance slit is oriented vertically, so one can perform constant energy maps by rotating the manipulator. One unique aspect of FinEstBeAMS is a minimum photon energy of 4.5 eV, compared to the 10 eV, 30 eV and 40 eV at Bloch, MAXPEEM and FlexPES respectively.

FlexPES is a multi-purpose beamline sourced by a linear undulator. It has two branch lines, one of which has a permanent endstation dedicated to XPS and XAS measurements of solid state samples. FlexPES has recently upgraded to a DA30 deflection analyzer. At present the analyser slits are horizontal and the vertical 4-axis manipulator is equipped for liquid nitrogen cooling.

MAXPEEM is photo-electron microscopy beamline. The endstation hosts an aberration-corrected SPELEEM microscope (Elmitec GmbH). With this instrument it is possible to perform micro-ARPES - however the energy resolution is currently limited to 100 meV. An upcoming upgrade is expected to improve this to 30-50 meV.

Beside these three beamlines, there is an ongoing effort to implement a soft X-ray ARPES (SX-ARPES) facility by constructing a movable endstation and bringing it to the B-branch of the Veritas beamline at the 3 GeV ring of MAX IV. The energy range of Veritas beamline is 275-2000 eV. The Bloch team is involved in this project, and initially it will reuse the R4000 analyser from the retired spin ARPES beamline (i3) at the previous generation MAX-Lab facility. The initial tests are quite encouraging. The SX-ARPES project is being pursued in collaboration with Prof. Oscar Tjernberg from KTH university in Stockholm.

2.5.2 ARPES facilities internationally

In Figure 13 we attempt to summarize the main characteristics of dedicated ARPES beamlines around the world. We consider only 'general' ARPES facilities here, and so do not include time-resolved or nanoARPES facilities.

Comparing different beamlines is a non-trivial task as there are many orthogonal axes one might choose for comparison, each one being important for some specific subset of user experiments. For the purposes of this discussion it is interesting to highlight 3 aspects:

Small spot size The spot size at the sample position at Bloch is $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m}$ at normal incidence. Comparing this with the much larger spot sizes available at most other facilities illustrates why it has been such a defining characteristic of Bloch so far, and the main attractions for much of our user community. However it is also clear this position won't be maintained forever; comparable spot size are reported at facilities such as Alba (LOREA beamline), NSLS-II (ESM-ARPES), SIRIUS (SAPE) and ALS (MAESTRO: microARPES) and we anticipate that most upgrade programs or new facilities will include small spot sizes.

Lowest sample temperature This we see as one of the major weaknesses in the Bloch beamline performance, which otherwise is highly competitive in terms of spot size, energy resolution, flux and possibility of changing photon beam polarisation. The lowest temperature at Bloch is about 15 K, reached at the B-branch. As one can see from Figure 13 there are indeed several beamlines that offer base temperatures of 10 K or better.

SARPES Also apparent from Figure 13 is that there are not many beamlines providing 3D spin-resolved ARPES measurements. We are in the process of commissioning the 3D VLEED equipped SARPES endstation at Bloch. Combined with the small spot size, the high flux reachable using the 92 l/mm grating and eventually the well characterized photon polarization we expect Bloch to be highly competitive for SARPES studies in future.

Facility	Country	Beamline	Endstation	Photon energy range	Spin?	Manip axes	Flux [ph/s] @ 0.1% BW	Spot size ($\mu\text{m} \times \mu\text{m}$)	Min. temperature (K)	Deflection	Other facilities
ALBA	Spain	BL20 (LORE)		10 - 350 (1000)		6	1e13	13 × 13	7.5		
SLS	Switzerland	X09LA (SIS)	ULTRA	20 - 800	planned	6	2e13 (200eV)	50 × 100	4	✓	
SLS	Switzerland	X09LA (SIS)	COPHEE	20 - 800	3D Mott	6	2e13 (200eV)	50 × 100	15		
SOLARIS	Poland	UARPES	UARPES	8 - 100				270 × 30	8		
SOLARIS	Poland	PHELIIX	PHELIIX				>1e13	100 × 100			
SOLEIL	France	CASSIOPEE	HR-ARPES	8 - 1500		6	2e13	40 × 20	13	✗	
SOLEIL	France	CASSIOPEE	Spin-resolved PES	8 - 1500	2D Mott	4		250 × 200	25	✗	
ASTRID-II	Denmark	SGM3	SGM3	12 - 150		6	2e13 (40eV)	120 × 30	30	✗	STM
BESSY-II	Germany	UE112_PGM	One cubed	4 - 200		6	>1e13	250 × 40	1	✓	
BESSY-II	Germany	UE112_PGM	One squared	9 - 250		6	>1e13	150 × variable	15	✗	
BESSY-II	Germany	UE125_PGM	RGBL2	15 - 200	2D Mott	6	>1e13	68 × 25	40	✗	
BESSY-II	Germany	[Movable]	Phoenix	...	2D Mott	5			
DLS	UK	i05	HR-ARPES	18 - 240		6	...	50 × 50	10	✗	
ELETTRA	Italy	VUV		20 - 750		5		500 × 100	9	✗	
ELETTRA	Italy	APF-E		10 - 100	3D VLEED	4	7e13	150 × 50	15	✓	STM, PLD
ELETTRA	Italy	BADeph		5 - 40		5		300 × 10	10	✗	
CLS	Canada	qmic	ARPES	15 - 1200			>1e12	20 × 100	9	✗	
CLS	Canada	qmic	SPIN-ARPES	200 - 1200	Yes		>1e12			✓	
UVSOR	Japan	BL7U (SAMRAI)		6 - 40		5		200 × 50	3.8		
UVSOR	Japan	BL5U		20 - 200		6	<1e12	23 × 40	6		
HSRC*	Japan	BL-9A		4 - 35		6		30 × ?			
HSRC*	Japan	BL-9B	ESPRESSO	16 - 80	3D VLEED	6					
HSRC*	Japan	BL-1		16 - 300							
NLS-II	China	21-ID-1 ESM		20 - 1500		4	1e11	900 × 200	11	✓	
SSRF	China	BL09U (Dreamline)	ARPES	20 - 200 (2000)		6	3.5e11 @ 0.01, 800eV	20 × 30	12	✓	STM, VUV laser
SSRF	China	BL03U		7 - 165		6		8 × 67	7	✓	
MAX-IV	Sweden	Bloch	ARPES	10 - 220 (1000)		4		10 × 10	19	✓	STM
MAX-IV	Sweden	Bloch	SPIN	10 - 220 (1000)	3D VLEED	4		10 × 10	15	✓	
LML5 (Sirius)	Brazil	SAPE		8 - 70		6	1E+12	20 × 20	16		
ALS	USA	4.0.3 (MERLIN)		10 - 150		6			10	✗	
ALS	USA	7.0.2	microARPES	20 - 1000		6	3e12 at 65eV	10 × 12	15	✓	
ALS	USA	10.0.1.1	HERS	17 - 350			1e13 at 0.01%, 30eV	100 × 100			
ALS	USA	10.0.1.2	spin-ARPES	17 - 350	3D VLEED			50 × 50		✓	
SSRL	USA	BL5-2		25 - 200		6		40 × 10	<10	✓	
SSRL	USA	BL5-4		7 - 40		5		100 × 00	5	✗	

Data are according to public website information on 28/04/2022, compiled as a best effort (errors possible)
* according to international review on 2018

Figure 13: Key specifications of synchrotron ARPES facilities.

3 User operation

3.1 User statistics

For the six initial years of operation of MAX IV, the aim is to make 75% of the beamtime at each beamline in full operation mode available to general users through a peer-reviewed proposal system, with the remaining 25% split between maintenance, commissioning, in-house research and collaborative research with groups that were involved in the build up of the beamline. For Bloch the latter case principally involves two user groups, from Linköping University and KTH. MAX IV runs a program for proprietary research (e.g. private industry), but to date Bloch has not received applications for this.

Beamtimes at Bloch are allocated in 30-shift, 5-day blocks (Wednesday-Sunday inclusive), with Mondays reserved for the accelerator group and Tuesdays dedicated to beamline and insertion device commissioning and maintenance. Beamtime allocation at Bloch can be divided into three categories:

General user program: General users are awarded beamtime in the standard peer-review fashion twice per year. Excepting some anomalies during COVID-19 pandemic (i.e. between June 2020 to September 2021), the fraction of awarded beamtime to the general user program has been steadily increasing as more functionality of the beamline has been made available through in-house and expert commissioning.

In-house user program: The in-house program encompasses development, commissioning, maintenance and scientific research, across the beamline and the two endstations.

Expert commissioning program: Refers to a selected number of shifts accessed through a special user call for 'expert commissioning' and dedicated to the testing of new infrastructure developed at the beamlines, before it is offered for the general user operation. These proposals are aimed at collaborative work with external user groups and are evaluated foremost on how the project will benefit the beamline.

3.1.1 Beamtime and proposal statistics

The Bloch beamline received light early 2018 to the ARPES endstation (A-branch). Bloch had the first expert commissioning users in February 2019 and first general users in August 2019. Table 4 summarizes the submitted and accepted proposals per proposal call.

	HT18 ¹	HT19	VT20	HT20	M-21	VT22 ²	Fall22 ²
Submitted	11	17	21	16	22	21	32
Accepted	5	9	9	9	7	11	11 ³
Oversubscription	2.2	1.9	2.33	1.78	3.14	1.91	2.9

¹ Commissioning period for ARPES endstation

² Commissioning period for spinARPES endstation

³ Anticipated; PAC has not yet met at time of writing

Table 4: History of submitted and accepted proposals

The COVID-19 pandemic resulted in a significant scheduling disruption due to both the MAX IV shutdown and the travel restrictions. Importantly, while this caused a great deal of rescheduling there were no cancellations. While proposals were not always scheduled in the cycle for which they were accepted, and the rescheduling demanded a reduced acceptance rate for subsequent cycles, all accepted proposals were performed owing to the creation of an efficient remote operation mode. Table 5

summarizes the beamtime use, and demonstrates this disruption. Time that became available due to rescheduling was used to better characterize the beamline and bring more instrumentation online.

	HT18	HT19	VT20 ¹	HT20 ²	VT/HT-21	VT22 ³	Fall22
Expert commissioning	11	0	0	0	0	1	2 ⁴
In-house	7	6	12	7	10	3	2.5
General	0	9	3	7	16	10	11 ⁴
Total	18	15	17	14	26	14	15.5
General share	-	60%	17%	50%	62%	77%	71%

¹ COVID-19 travel bans begin

² First remote beamtime

³ Operation back to 'normal'

⁴ Anticipated; PAC has not yet met at time of writing

Table 5: Division of beamtime at Bloch

Remote operation: When COVID-19 travel bans began taking effect and preventing users from departing and/or arriving to Sweden, it quickly became apparent that some form of remote operation would be required for Bloch to maintain sufficient scientific output and connection with the user community. Due to a combination of factors, Bloch was able to roll this out quickly and to good effect: many of our user experiments are relatively well suited to remote access ('cleave and measure'), the beamline team feels very strongly about making maximum use of all available beamtime, and remote-desktop software has become very good in recent years. Of the 12 user beamtimes that ran in 2020, 10 were conducted by remote access. Now that travel bans have lifted, we no longer see fully-remote beamtimes but a hybrid mode of operation continues (part of the user team comes in person, others 'call in' to assist). We anticipate that this will continue indefinitely.

Recurring users: Of the initial 50 experiments, only 46% were from returning users. On one hand this puts a high load on the beamline staff who have to spend considerable time training new users, but at the same time this is an encouraging indication of a growing user community.

Nationality: Of the initial 50 experiments at Bloch, 42% had links to Swedish universities, 34% to other European institutes and 24% from outside Europe. MAX IV has no policy regarding quotas for local users; all proposals are evaluated by the PAC on equal footing.

3.1.2 User feedback

Through official channels, after each beamtime the user is offered to leave feedback on all aspects of their experience and the facility (e.g. user office services, uptime, IT systems, scientific support...). The averaged user feedback acquired through formal channels has been very positive (>90%) as the beamline and beamline infrastructure has matured since the first experiments in 2018-2019. However we often find that more honest and actionable feedback is obtained by offline discussion with the users. Towards the end of each beamtime, the beamline team makes an effort to solicit feedback informally, through which we get very useful information that informs our development plans.

3.1.3 Publications

As of this review (May 2022) there are 17 accepted journal articles that resulted from work performed at the Bloch beamline. Unsurprisingly, the time from experiment to a published article can sometimes exceed 3 years. so it will take quite some time before the output will reflect the actual productivity of

the beamline. The average impact factor is high, but also skewed by outliers in high impact Nature journals.

Cycle	# Publications to date	Impact factors
HT18	3	11.2, 11.2, 14.9
HT19	5	4.0, 4.0, 8.2, 9.2, 50.0
VT20	4	4.0, 4.0, 4.1, 6.5
HT20	3	(TBD) ¹ , 18.8, 43.8
VT/HT 21	2	7.3, 14.9
VT22	0	

¹ 'Physical Review Research' impact factor not yet determined

Table 6: Publications arising from beamtimes at Bloch

Bloch publication list

- [1] Ilya Belopolski et al. "Observation of a linked-loop quantum state in a topological magnet". In: *Nature* 604.7907 (Apr. 2022), pp. 647–652.
- [2] Dmitriy A. Chareev et al. "Growth of Transition-Metal Dichalcogenides by Solvent Evaporation Technique". In: *Crystal Growth and Design* 20.10 (Aug. 2020), pp. 6930–6938.
- [3] A. V. Fedorov et al. "Insight into the Temperature Evolution of Electronic Structure and Mechanism of Exchange Interaction in EuS". In: *The Journal of Physical Chemistry Letters* 12.34 (Aug. 2021), pp. 8328–8334.
- [4] Hrag Karakachian et al. "One-dimensional confinement and width-dependent bandgap formation in epitaxial graphene nanoribbons". In: *Nature Communications* 11.1 (Dec. 2020).
- [5] Hrag Karakachian et al. "Periodic Nanoarray of Graphene pn-Junctions on Silicon Carbide Obtained by Hydrogen Intercalation". In: *Advanced Functional Materials* (Jan. 2022), p. 2109839.
- [6] Igor Marković et al. "Electronically driven spin-reorientation transition of the correlated polar metal $\text{Ca}_3\text{Ru}_2\text{O}_7$ ". In: *Proceedings of the National Academy of Sciences* 117.27 (June 2020), pp. 15524–15529.
- [7] Max Mende et al. "Strong Rashba Effect and Different f d Hybridization Phenomena at the Surface of the Heavy Fermion Superconductor CeIrIn_5 ". In: *Advanced Electronic Materials* 8.3 (Dec. 2021), p. 2100768.
- [8] Thi Thuy Nhung Nguyen et al. "Topological Surface State in Epitaxial Zigzag Graphene Nanoribbons". In: *Nano Letters* 21.7 (Apr. 2021), pp. 2876–2882.
- [9] J. R. Osiecki, S. Suto, and A. Chutia. "Periodic corner holes on the $\text{Si}(111)$ - 7×7 surface can trap silver atoms [just accepted]". In: *Nature Communications* (2022).
- [10] Yu Pan et al. "Giant anomalous Nernst signal in the antiferromagnet YbMnBi_2 ". In: *Nature Materials* 21.2 (Feb. 2022), pp. 203–209.
- [11] S. Schulz et al. "Classical and cubic Rashba effect in the presence of in-plane 4f magnetism at the iridium silicide surface of the antiferromagnet GdIr_2Si_2 ". In: *Physical Review B* 103.3 (Jan. 2021).
- [12] J Shah et al. "Experimental evidence of monolayer arsenene: an exotic 2D semiconducting material". In: *2D Materials* 7.2 (Feb. 2020), p. 025013.
- [13] Jalil Shah et al. "Atomic and electronic structures of the Au_2Sn surface alloy on $\text{Au}(111)$ ". In: *Physical Review B* 104.12 (Sept. 2021).

- [14] Shangjie Tian et al. “Magnetic topological insulator $\text{MnBi}_6\text{Te}_{10}$ with a zero-field ferromagnetic state and gapped Dirac surface states”. In: *Physical Review B* 102 (July 2020).
- [15] Zhongzheng Wu et al. “Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu_2Si_2 ”. In: *Physical Review Letters* 127.6 (Aug. 2021).
- [16] Xiàn Yáng et al. “Observation of sixfold degenerate fermions in PdSb_2 ”. In: *Physical Review B* 101.20 (May 2020).
- [17] Hemian Yi et al. “Surface charge induced Dirac band splitting in a charge density wave material $(\text{TaSe}_4)_2\text{I}$ ”. In: *Physical Review Research* 3.1 (Mar. 2021).

3.2 Staffing

The Bloch team consists currently of five permanently employed beamline scientists, one temporary employed beamline engineer and two postdocs hosted here through external collaborations. Four of the scientists have a long history of running and operating the two predecessor ARPES beamlines i3 and i4 at the MAX III ring prior to its shutdown in 2015. These four were also responsible for planning and delivering the Bloch beamline project, although here two additional people outside the beamline team must be acknowledged: Rami Sankari was the principal designer of the beamline optics, and Roger Uhrberg of Linöping University is the beamline spokesperson and was heavily involved with the design and procurement of the A-branch endstation.

Balasubramanian (Balu) Thiagarajan (Beamline scientist, permanent) Beamline scientist at MAX IV since 1997. Participates in user support and local contact duties.

Mats Leandersson (Beamline scientist, permanent) Beamline scientist at MAX IV since 2000, manager of predecessor SARPES beamline i3. Participates in user support and local contact duties.

Craig Polley (Beamline manager, permanent) Joined the predecessor ARPES beamlines i3 and i4 as a postdoc in 2013. Became a permanent beamline scientist in late 2018, and assumed the beamline manager role from Johan Adell in 2021. Participates in user support and local contact duties.

Gerardina (Dina) Carbone (Beamline scientist, permanent) Joined the Bloch team in 2019 after five years at the NanoMAX beamline at MAX IV. New to ARPES but extensive experience with diffraction and coherence techniques, beamline operation and user support. Participates in user support and local contact duties.

Johan Adell (Beamline scientist / Group manager, permanent) Beamline scientist, previously beamline manager of predecessor ARPES beamline i4 as well as at Bloch. Now promoted up to group manager role for ‘Spectroscopy 1’, but still maintains a presence in the beamline team.

Jacek Osiecki (Research engineer, temporary) Joined the Bloch team in late 2021 but has prior experience as a beamline scientist at the soft X-ray photoemission I311 on the MAX-II ring. Participates in user support and local contact duties.

Hanna Fedderwitz (Research engineer, temporary, KTH employee) Was a Bloch postdoc during 2018-2020. Still stationed at MAX IV and informally hosted by Bloch, but now employed temporarily by Oscar Tjernberg at KTH University, until June 2022, to drive the development of a movable soft X-ray ARPES endstation at the Veritas beamline.

Khadiza Ali (Postdoctoral researcher, temporary, Chalmers employee) Joined in 2021 as a postdoc in Saroj Dash’s group at Chalmers University in Göteborg. Pursuing an independent research program on 2D quantum materials and also collaborating extensively with current and potential future users. Participates in user support.

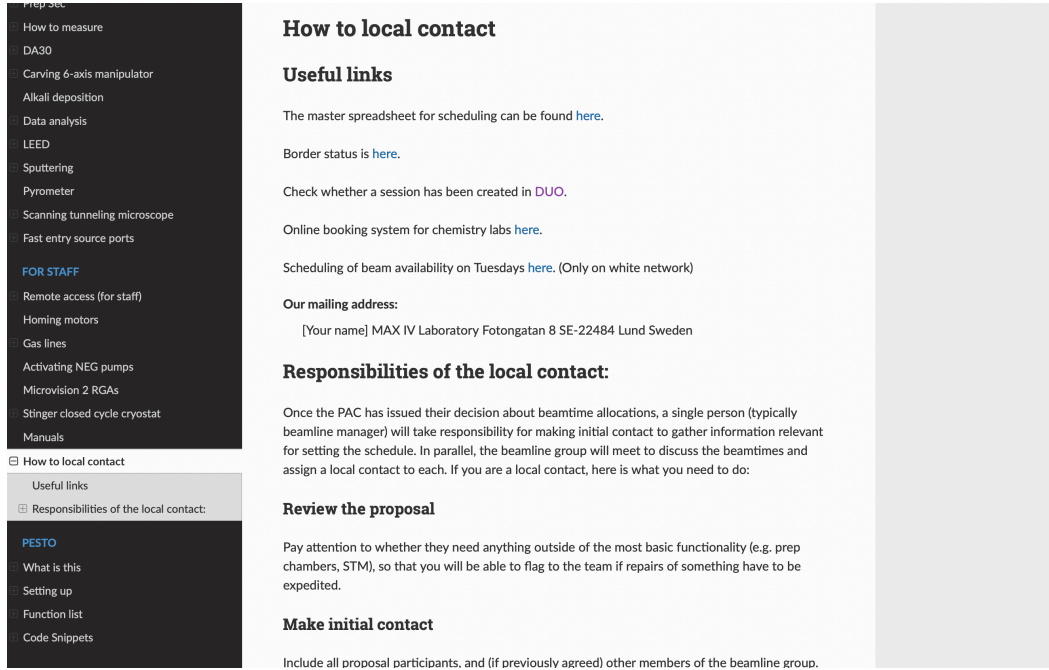


Figure 14: Internal documentation page codifying tasks and responsibilities for local contacts

3.3 Typical beamtime process

Beamtime allocation Proposal rounds at MAX IV occur twice per year, and the allocation of available beamtime follows a protocol that is uniform across the facility. After the beamline team performs a basic technical feasibility check, all proposals are sent for scientific review to the program advisory committee (PAC). Accepted proposals are then scheduled at the beamline; at Bloch all proposals are given five days of beamtime. The beamline manager takes the responsibility of coordinating the technical feasibility checks and the allocation of beamtime to the users. Once a beamtime has been scheduled, further coordination becomes the responsibility of a local contact (LC) from the beamline team. All members of the team participate in both LC and on-call (OC) duties on a week-by-week basis. LC assignment is based on availability during the scheduled week, the specific interest towards the proposal’s topic and/or a history of previous collaborations with the user group.

Local Contact responsibilities The LC assumes responsibility for providing a smooth experience for users at the beamline, and also acts as a single point of contact to the user group. To make the process both easier and more standardised, Bloch has a check list that every local contact can follow (Figure 14). Namely, a few weeks before the beamtime, the LC makes contact with the users to:

- advise them of their point of contact at the beamline
- check and confirm all experimental details described in the proposal, establishing whether any special preparations need to be made at the beamline

- inform about logistics (travel, accommodation and food) and inform about remote access options
- guide them through MAX IV administrative and safety requirements

Closer to the scheduled beamtime, the LC takes care of:

- arranging VPN credentials if needed and instructing users on the mechanics of remote access
- ensuring that all equipment needed for the experiment is in place and in good working order
- arranging safety training sessions for those who need access to chemistry labs for sample preparation
- coordinating with other members of the beamline team to ensure that the users will have the in-person help they will need throughout the week

User experience The standard length of a beamtime at Bloch is five days (Wednesday 0800 to Monday 0800). Users working on site normally arrive on the Monday or Tuesday preceding their beamtime to start the sample preparation, take their safety training and get familiarized with the beamline. The support of the users, that can include several members of the beamline staff, can be more or less involving, depending on the users experience and complexity of their proposal. Typical user support tasks during a beamtime include:

- training of users on the basics of the experimental station (safety, sample transfer, auxiliary equipment) & control software
- basic support to start the measurements (scientific and technical assistance with the first phases of the user's experiment) & data visualization using beamline software
- for inexperienced groups, working closely with the users to achieve and sometimes define their experimental plan
- providing a continuous support channel during working hours and arranging an out-of-hours support channel (typically a messaging client like WhatsApp or Slack)
- ensuring all samples and sources are removed at the conclusion of the beamtime
- at the next team meeting following the beamtime, briefly discuss the results obtained, the problems encountered and the feedback offered by the users.

A formal OC support system exists that covers 1700-2300 on weekdays and 0800-2000 during the weekend. However, usually, the first two days of the beamtime the local contact stays with the users until needed, even beyond working hours, gradually exploring all the features of the end station according to the experimental plan. Furthermore, a continuous support channel is offered for support after working hours through a messaging client. This tends to supplant the use of the OC phone system, with the benefit of being asynchronous and greatly increasing the availability of support by simply increasing the number of people that can be reached at any given moment. We have also found that due to the complexity of the beamline and the large variety of equipment present, the detailed knowledge of all details is rather diffuse within the team. Therefore, it is quite common that more than one person is needed to answer all the technical and scientific requests of the users.

With the aim to both improve the user experience and to reduce the support load on staff to sustainable levels, large and ongoing efforts are directed towards reducing the complexity of the user interface and also proving comprehensive beamline documentation (see Section 6.2)

Facility support There is also on-call support available at the facility level to both users and to beamline staff during non-office hours, from all major divisions in the laboratory (e.g. accelerator, IT, PLC, experimental safety...). In addition to this a program of staffing 24/7 on-site 'floor coordinators' has recently begun, aiming to provide a constant, centralized point of contact for both users and staff.

3.4 Growing the community

In order to increase the user community we take different actions, that can be grouped in three main categories: basic scientific outreach, collaborations/outreach to Swedish universities and education.

- **Basic outreach** This includes a number of actions that are typical to similar facilities:
 1. The existing user community's publications and their network. We already notice that more new users learn about Bloch through this channel and are applying for beamtime.
 2. Occasional seminars on ARPES at SciencifiKa¹, a weekly seminar series organised by MAX IV Laboratory for its user community.
 3. MAX IV Users Meeting sessions dedicated to ARPES, often inviting potential new users and/or presenting potential new developments.
 4. Co-organisation or active support of workshops. Most recently a successful workshop was co-organised in 2021 with KTH in Stockholm, mainly aimed to widen the ARPES community in Sweden involved in quantum materials.
 5. Presenting the beamline and its results at conferences.
- **Collaborations** : Post-docs paid from Swedish Universities are placed at Bloch, to pursue a specific research plan. They participate to the beamline activities and can be involved in user operation, if they are interested.
 1. Chalmers University of Technology (Chalmers): We have an active ongoing collaboration with Prof. Saroj Dash, who is an expert on quantum devices. A postdoc (Khadiza Ali) is stationed at Bloch for research activities and the development of transport and spin-resolved STM. Apart from the work with the Dash group, this collaboration helps to reach out to other groups in Chalmers.
 2. KTH University, Stockholm: We have an active collaboration with Prof. Oscar Tjernberg, who has interest in both the Bloch and Veritas beamlines. We presently have one postdoc (Hanna Fedderwitz) stationed at MAX IV. She is presently setting up a soft X-ray ARPES endstation, which is currently being tested on Veritas B-branch.
 3. Single measurements / feasibility checks: We informally offer to current or potential users that they may leave samples with us and if an interested team member is available when unforeseen free time arises (e.g. commissioning work finishes early), we will attempt to perform short feasibility tests or complete missing measurements from a dataset. This can have a variety of benefits for us such as initiating longer term research collaborations, allowing inexperienced new users to write much stronger proposals or permitting current users to easily answer referees and publish data from Bloch. In the near future we intend to formalize this system by participating in the Fast Access program offered by MAX IV.
- **Education outreach** : Includes all activities where students are directly involved, either to develop a supervised research plan or to participate in training activities.
 1. Masters students: one student has obtained her Master (Anita Shah) from Lund University based exclusively on work performed at Bloch. Her thesis title is "Characterizing the energy resolution of Bloch beamline" (<https://lup.lub.lu.se/student-papers/search/publication/9024713>). We plan to continue to support Master student thesis projects.

¹<https://www.maxiv.lu.se/science/scientifika/>

2. Beamline staff as co-supervisors for Ph.D students: MAX IV has initiated a funding plan for Ph.D students with main supervisors from Swedish universities and MAX IV staff as co-supervisor. Craig Polley is involved in a Ph.D project proposal from Karlstad University and Balasubramanian Thiagarajan is involved in a proposal from KTH. Acceptance of the proposals is not confirmed at the time of writing.

3. Hands-on experimental sessions: One of us (Balasubramanian Thiagarajan) teaches a masters course at Lund University, that includes a one-day experimental session where students get an experience of the measurements or ARPES at the beamline. Furthermore, we supervise and support hands-on experiments of university students, through the education beamtime proposal plan recently started at MAX IV.

4 User and in-house research

At present the 'gold-rush' for discovering topologically nontrivial materials is still going strong, and Bloch receives many such proposals particularly given that the small spot size is useful for studies of difficult crystals that may be very small or not cleave well. While proposals like these tend to be productive in terms of high impact publications, our program advisory committee has been mindful of the need to maintain a diverse balance of proposals. Examples of other projects capitalizing on the small spot include exfoliated flakes, crystals with multiple surface terminations and applied strain gradients. In general there are four factors that are common to most proposals: the small spot size, the deflection analyzer, the ability to measure over a wide temperature range and of course the high flux, high resolution beam standard to a modern synchrotron beamline. During the in-person review there will be presentations from two of our repeat user groups (Phil King and Denis Vyalikh) who will present some of their work and explain from their perspectives what the strengths (and weaknesses) of Bloch are.

The in-house research program at Bloch is close to an equal mixture of individual research interests and collaborations with users groups, and will be summarized in dedicated presentations during the in-person review. Since coming on-line, Bloch has dedicated an increasing number of shifts to user operation, while still investing a fair amount of time in commissioning and development activities. Therefore, the line between beamline development (optimisation, user collaboration and in-house research) is often blurred.

5 Known deficiencies

Before embarking on the discussion about ongoing development work in Section 6, it is worth first highlighting known deficiencies of Bloch. These are defined as things that do or may result in Bloch underperforming relative to *baseline expectations*. In most cases, a solution has been at least identified.

5.1 Carving manipulator: temperature, robustness, motion cross-talk

The 6-axis Carving manipulator on the A-branch endstation was modified from the base design by Specs (at our request) to permit electrical current to be passed through the sample at a specific azimuthal angle. This was originally envisaged to allow easy direct-current annealing of samples without transferring to the preparation chambers. An additional, and unexpected, application has been measuring ARPES spectra while passing a small current through the sample to drive a phase transition.

In practice, both these features have been very rarely used, while the compromises to the robustness and strength of sample clamping have impacted most users. We believe that the resulting inadequate thermal contact is a major contributor to the sample base temperature of only 19 K, which has become the least appreciated feature for the users, since 10-15 K is offered at most other comparable facilities. The clamping accomplished in this design has a very tight thickness tolerance and several experiments have been disrupted by an inability to clamp (or release) a sample plate. We believe it would be possible to rebuild the sample receiver in future with a relatively non-invasive modification, removing the electrical contacts in favor of a stronger and more robust sample clamping. This could be done in-house with relatively minor engineering work, and would likely bring us closer to a sample temperature of 15 K. It would remain possible to revert to the original configuration if needed for a particular experiment. As will be discussed in section 6, today there are several options for high-performance commercial or in-house manipulator designs. If there is a strong call for even lower temperatures and higher performance, this is one of the few areas where money alone would suffice to fix it.

Aside from these considerations, more work needs to be done to improve the stability and reproducibility of the manipulator motions. This is particularly true given the small spot size and the growing number of experiments that rely on it. Here the worst offender is the polar motion, which couples in very large (mm) linear displacements when changing direction. Similarly, changing direction in the vertical y-axis couples in a small but noticeable displacement in the horizontal x-axis. While it is possible to largely mitigate these effects with software backlash compensation, it would be far preferable to find and eliminate the mechanical source. Today the origin is still unclear to us, and ultimately the solution will likely involve adding an *in-situ* support collar around the support tube.

5.2 Spectrometer control software

On the A-branch the spectrometer is controlled with the default SES software package offered by Scienta, with limited control of the sample (position and rotations) and photon beam (energy) parameters. It is unaware of and other important parameters (e.g. sample temperature, slit settings,...). This solution is only barely sufficient for user operation, as there are several limitations it imposes:

- **File formats and metadata:** Data can only be saved in 2 file formats, and currently only a small subset of the beamline configuration is included in the metadata. It would be far preferable to support a wider range of formats (including e.g. NeXus [1]) and to record all available metadata such as sample temperature and beamline settings.
- **Stability:** SES is has a reputation for unusual crashes, and disruptions and data losses are not uncommon.
- **Interlocks:** There is currently no available mechanism to interlock against excessive intensity on the MCP, which leads to ‘transmission stripes’ being burned into the detector response. We

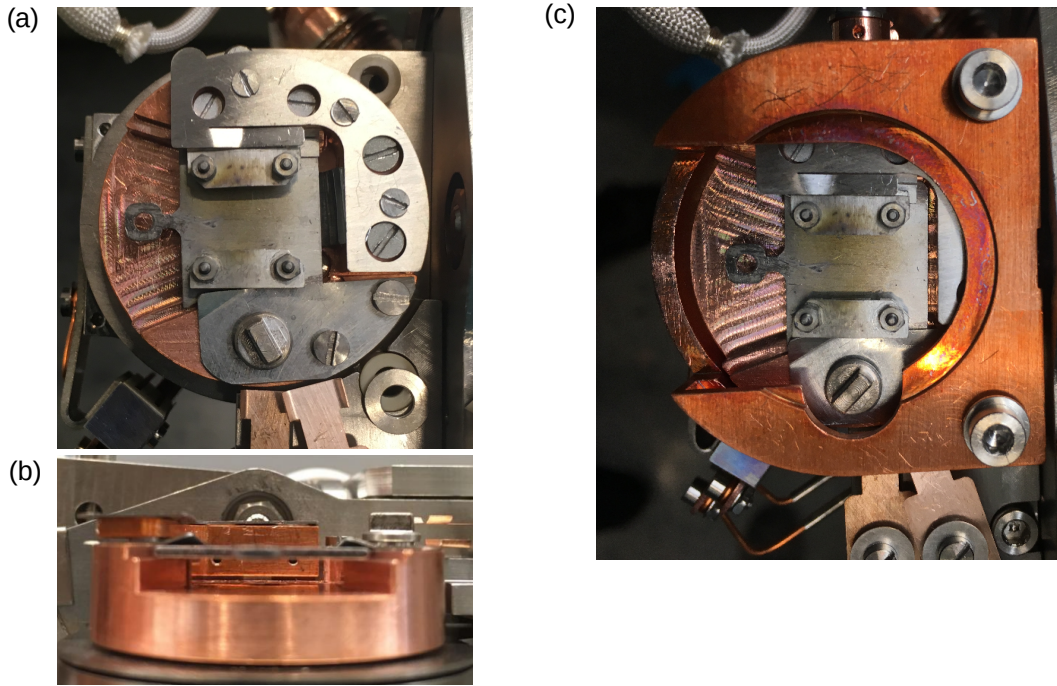


Figure 15: The customized Carving receiver delivered by Specs. With the cryoshield removed (a,b) it is clear that thermal contact between the sample plate and the stage is poor - plates are only contacted on two edges, and only one of those edges is mechanically clamped by a tightening screw. The cryoshield (c) provides only minor coverage of the sample, and due to extremely tight tolerances there are frequently issues with the receiver contacting or even seizing against it during azimuthal rotations.

rely on users being careful and diligent about respecting count-rate limitations. This is a case of misaligned incentives, since we want the MCP to remain homogeneous for all users, while any given group wants to maximise the output of their particular experiment. An intensity interlock would immediately realign our incentives.

- **Sophisticated measurement sequences:** It is currently not possible to automate certain measurements such as circular dichroism or temperature dependent ARPES. This results in many users having to manually perform tedious data collection in cases where it could and should be completely automated.
- **Sophisticated measurement types (e.g. dither mode, fast raster scanning):** The field-terminating mesh in front of the MCP means that images acquired in fixed-mode contain an undesirable background. With more advanced spectrometer control it would be possible to implement 'dither'-type measurement modes that preserve the valuable efficiency advantage of fixed-mode measurements while largely eliminating the mesh. It would also be possible to implement much faster manipulator raster scanning during spatial maps, which is proving to be an important technique to take advantage of the small spot size.

One possible solution to this is to build a custom control interface using the *SESWrapper* provided by Scienta [2]. To date this has not been explored owing mainly to a lack of resources and relevant expertise. A second solution has recently emerged with the launch of Scienta's new PEAK software, which replaces SES. This will be a large undertaking, but Bloch is actively working to migrate to PEAK and we are hopeful that this can be completed and all the aforementioned issues solved within

12-18 months.

5.3 Heat-load deformations of M1

The pitch of the M1 mirror deflects the beam horizontally. Given perfect alignment, there should be a single optimal value of M1 pitch that maximises flux on the sample. In reality, certain deficiencies in the M1 mirror chamber design (from FMB-Berlin) have led to a heat-induced distortion issue whereby the M1 alignment can change as a function of time. This often leads to measurements being performed with sub-optimal countrates, and makes working at low photon energies (<20 eV) more challenging as the drift requires several hours to stabilize.

This problem affects several beamlines at MAX IV. Working in collaboration with FMB, a design modification has recently been deployed at the Veritas beamline and is showing great promise. We are optimistic that we can deploy a similar modification at Bloch and this will largely solve our M1 stability issues.

5.4 Mirror corrosion

Bloch, along with several other beamlines at MAX IV, uses Toyama monochromators with In-Sync M2 mirrors. There have now been two instances (Veritas and SoftiMAX beamlines) where corrosion of the water cooling connectors has nearly resulted in the need to procure a new M2 mirror, which would halt the operation of the beamline for several months. There is currently not an agreed-upon cause nor solution to this. While this presents a risk of future downtime if corrosion begins at Bloch, user operation is at present completely unaffected. We monitor closely for early indications of corrosion and work is ongoing at the facility scale to understand and address the issue.

5.5 Difficulty of access

As the oversubscription ratio grows at Bloch, so does the barrier to new users, particularly those with risky or unproven samples who may develop into power users if given a chance. The present solution to this is an informal standing offer for users or prospective users to send samples to us at the beamline (as described in Section 3.4 above), to be attempted if short windows of free time come up at short notice on a best-effort-no-promises basis. There are a multitude of inadequacies with this approach. The formal solution to this at MAX IV is in the form of fast-access proposals, where users can apply for 12-24 hour beamtimes to perform basic feasibility checks. Thus armed with preliminary data, they should be enabled to write much stronger proposals in subsequent calls. It is clear to us that Bloch will eventually join other beamlines at MAX IV in offering this, after careful consideration of how this might affect the workload on the beamline staff.

6 Beamline development

In this section we discuss development projects at the beamline that we are either actively working on or have concrete plans to spend time on in future. There is some overlap here with the deficiencies listed in the previous section; we take it as a given that those are all high priority items and will be addressed.

6.1 Commissioning of baseline capabilities

Although the beamline has been operational and taking users for over 3 years now, there remain aspects of the beamline that were specified in the original design but have not yet been fully commissioned and deployed. Before discussing *new* developments that are being worked on or considered, we first discuss these missing baseline features here. As the SARPES endstation has already been discussed at length, we do not mention it here but would highlight that it is nonetheless an ongoing project that is consuming significant resources.

6.1.1 Full use of the monochromator

As discussed in Section 2.1.2, the monochromator at Bloch is quite sophisticated, offering users the freedom to adjust c_{ff} , select between three different gratings in cPGM mode or reconfigure into a NIM mode. In reality, today users stay exclusively on the cPGM 800 l/mm grating at $c_{ff}=2.25$, so this flexibility is not being used. Besides the 92 l/mm and 2400 l/mm gratings being installed later (aligned and tested February 2020), there are two main reasons for this situation. Firstly we have optimized the user experience for this specific configuration (e.g. characterising flux and resolution and carefully maintaining an energy calibration better than 15 meV). The other gratings have been coarsely explored during in-house times, but more time investment is needed to improve the experience of using these alternative configurations. This will come naturally if we begin deliberately exploring these configurations ourselves during in-house projects, and the 92 l/mm grating will naturally rise in priority as the SARPES station comes online. Likewise, once the polarimeter project (see Section) takes off there will naturally be higher interest in working with the NIM operation mode. The second reason for the low prioritization of offering all monochromator modes has simply been the excellent performance of the 800 l/mm grating. For the user experiments so far there has been no strong need to switch modes, and users have valued the convenience of being able to conduct an entire experimental run on a single grating.

6.1.2 Higher order suppression

The original beamline design included a number of provisions for higher order suppression (discussed in Section 2.1.2). Between the quasiperiodic undulator, the adjustable baffles in front of all optical elements, the gas-cell built into the exit slits and the provision for solid state filters, there should be enough flexibility here to offer users whatever degree of higher order suppression their experiment needs. In reality, today it is extremely rare for users to even notice higher order contamination let alone be disturbed by it. Certainly the quasiperiodic undulator has helped in this respect. Absent any strong push from the users, it has been difficult to motivate prioritizing higher order purity. There is even some thought being given to removing the gas cell functionality from the A-branch exit slit, to reduce the complexity and maintenance requirements of a 6-turbo pump apparatus. Before committing to this we would first invest time characterizing how bad the higher orders are (across all monochromator modes), to what extent the baffles and solid-state filters alone can clean it up and carefully considering the strategic impact it would have on the beamline in future.

6.2 Usability projects

Technical excellence and a high uptime are necessary but not sufficient for an excellent facility - ultimately the purpose of a beamline is to take users as input and produce high quality publishable science as output. A crucial but sometimes overlooked ingredient here is enabling the users to ignore irrelevant details of the beamline operation and focus on accomplishing their scientific aims. Here we discuss five areas where there are specific and ongoing efforts at Bloch. These are things that don't necessarily represent large discrete projects but rather continuous, iterative background time investments.

6.2.1 Control scripts

The control system is the most obvious place where the user experience is made or broken, but is not always obvious whether and how things can be improved. Here Bloch has benefited a great deal from the **fast feedback loop** that results from using the beamline ourselves for research projects, noticing things that are annoying and then having competence within the team to create better interfaces and sophisticated pseudomotors without necessarily being reliant on external resource groups. Examples of this include:

- Axes for the measurement manipulator that include software bounding boxes. These can update depending on the task being performed, and in principle make it impossible for the users to ever do something like driving the manipulator into the analyzer
- Condensing common operations into single-button operations for the users (e.g. macros for venting the loadlock or moving the measurement manipulator along a safe path between transfer and measurement positions)
- A virtual photon energy control that transparently includes energy corrections, undulator settings for the desired polarization mode and mirror corrections.

In a similar way, the ease with which the Tango control system can be incorporated into python scripts has enabled Bloch to quickly test and deploy new control solutions (and importantly to iterate on those solutions). This was pivotal to our success at rapidly making productive remote-access beamtimes possible during COVID-19.

6.2.2 Analysis/visualization tools (*pesto*)

As Bloch went into operation, one of us decided to change from a workflow based on Igor Pro to one involving Python/Jupyter. This has culminated in a fairly comprehensive package (*pesto*) that we use heavily ourselves and make freely available to our users. There are tools for fast visualization, calculations and sample alignment that are appreciated by almost all user groups. While for most users don't need to go further with it into complicated data analysis (most already have a solution that they are more familiar and productive with), it means that we can offer a license-free solution to those that are new to ARPES and need tools to help them work with the data they collect. The current version is hosted on [gitlab](#), with documentation for the package at [pesto.readthedocs.io](#). In the immediate future this will need to be expanded to cover the data coming from the SARPES station.

6.2.3 Beamline manual (*BlochDocs*)

Continuous effort is invested to produce an authoritative, well organized single source of all important technical details about the beamline. We opted to create this in a popular markdown package (*sphinx* and *readthedocs*) instead of the standard MAX IV wiki packages for various reasons including readability, high reliability and the ability to easily access this information from off-site. It is currently being configured at a publicly accessible site, and by the time this report is published should be available at [blochdocs.maxiv.lu.se](#).

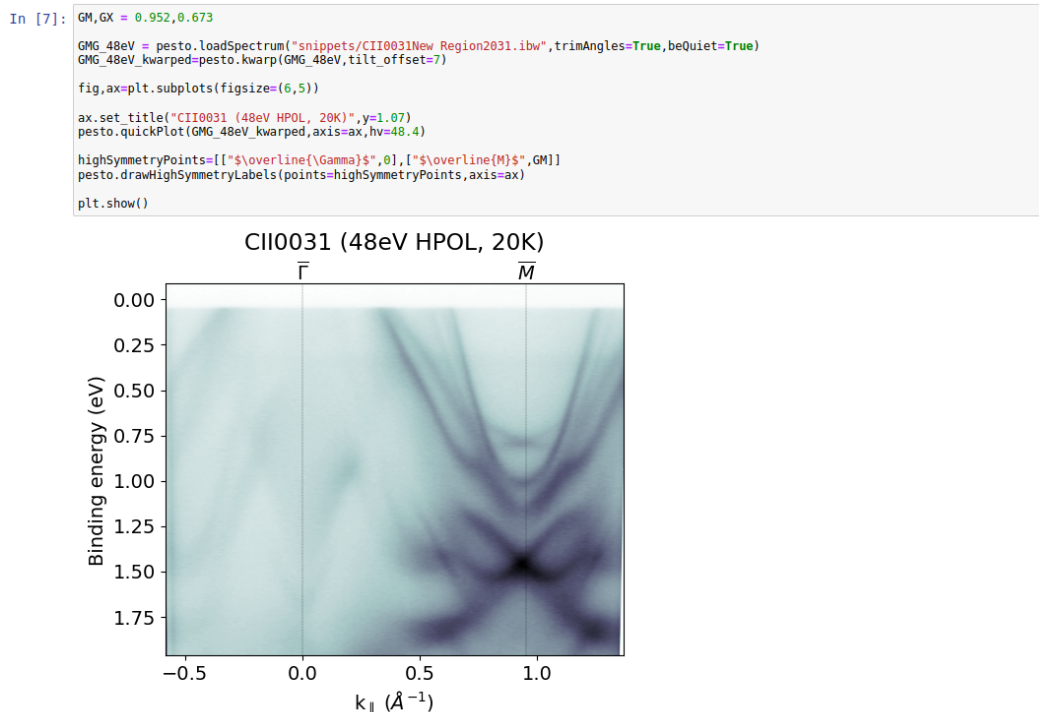


Figure 16: Example of data visualization with the *pesto* package

Search docs

FOR GENERAL USERS

- Sample mounting & cleaving
- Loadlock
- Prep Main
- Prep Sec
- How to measure at Bloch
 - Maximum countrate
 - Control GUIs
 - Optimizing flux
 - Using SES
 - DA30-L electron analyzer
 - Carving 6-axis manipulator
 - Alkali deposition
 - Data analysis
 - LEED
 - Sputtering
 - Pyrometer
 - VT-XA STM
 - Fast entry source ports
 - Getting your data
 - Manuals

How to measure at Bloch

Maximum countrate

Excessive countrates will damage the MCP in the detector assembly, and at BLOCH it is very easy to generate unsafe countrates. Respect the following rules:

1. Maximum 1 million counts/s if everything is in a narrow stripe (for example transmission mode or graphene's Dirac cone)
2. Maximum 10 million counts/s if intensity is evenly distributed across the detector
3. Core levels should be measured in an angular lens mode, except where lens table limits make this impossible.

Warning

There is no background process in SES to monitor countrates, so you must verify that the countrate is safe while in voltage calibration mode. If you will perform an angle scan or photon energy scan, check the intensity over the whole scan range, not just your starting position. If you will measure in swept mode, ensure that the intensity slightly below your starting point is also safe.

Control GUIs

How to launch control GUIs

For the control panels on the 'Scienta' spectrometer control computer (Windows), there is a folder

Figure 17: Beamline documentation pages (*BlochDocs*)

6.2.4 Spectrometer control interface

The upgrade from SES to PEAK on the A-branch has already been mentioned, but this will bring the ability to invent new, optimized user interfaces and measurement sequencers. Since the Prodigy control system on the SARPES branch is already configured for remote control, we can hopefully create a unified user interface across both endstations. This will be performed mostly within the Bloch team to enable rapid prototyping and iteration.

6.2.5 Electronic focus adjustments

A new development from Scienta-Omicron is the ability to electronically translate the focal point of the analyzer. The value of this is clear to us: we routinely see the situation where a user has a difficult multi-domain sample on which they have finally found a good part, only to learn that they are out of focus. In such a case one has to decide whether the improved measurement quality is worth the sometimes significant time cost of moving the manipulator to fix the focus. Scienta-Omicron is preparing to launch this as an upgrade in later 2022, and we have plans to collaborate with engineers there on the testing and development of the feature using the DA30L at Bloch.

6.3 Major development projections

6.3.1 Characterization and control of photon beam polarization

Insertion devices for low energy X-rays possess the intrinsic capability of producing photon beams with controlled polarisation, which is often useful and sometimes essential for scientific applications. Linear and circular polarisation of the light introduce new variables in the parameter space of the interaction of photons with matter that increase the quantity and quality of information that can be extracted through measurements. This is for example exploited in magnetic dichroism in the soft and hard X-ray range, where X-rays with opposite helicity are used to extract purely magnetic information from samples.

A complication introduced by low energy photons is the strong effect of the BL optics on the polarisation of the photon beam produced by the undulator. While for photon energies above 150 eV the effect of BL optics is irrelevant, below this energy the BL optics effects become dominant and assuming the same polarisation state at the sample as at the EPU is not sufficient. Therefore, a more sophisticated control of the EPU that allows compensating adjustments to the gap and phase setting is necessary to create circular light and purely linear inclined light *at the endstation*. This requires the deployment of a Universal Mode for the EPU and the development of characterisation tools at the endstation. These are included in two parallel projects started at Bloch in October 2020 and still ongoing. The first project coordinates efforts from the Software team, the Insertion Device team and the Accelerator group for (i) implementing the separate motion control of the EPU girders, (ii) commissioning the EPU motion and neutralising the related electron beam orbit and optics disturbances in the 1.5 GeV ring of MAX IV Laboratory. The second project involves the design and construction of a compact polarimeter, just completed at the time of writing and installed in the B-branch endstation, and the refinement of measurement schemes and analysis tools to characterise the polarisation of the beam at the sample position.

The modern interpretation of ARPES data, although quite well developed, strongly relies on theoretical models and band structure simulations which, in turn, are based on previous knowledge. It can therefore be quite difficult to extract completely new or unexpected information from measurements of new complex materials where a proper model is not available. A common approach to qualitatively single out contributions from different orbitals is to use incident light with different polarisation, e.g. linear horizontal or vertical and circular with opposite helicity. This helps to separate and highlight, in a mere qualitative way, different contributions to the material's band structure, by changing the intensity ratio between different components. A more quantitative approach to orbital decomposition

has not yet been developed due to the lack of well characterised beam polarisation in the low energy X-ray regime. By providing full control and proper characterisation of the polarisation of the light, Bloch has the possibility to uniquely develop this simple qualitative approach toward a fully quantitative one. This approach will allow benchmarking of models and theories of complex materials against quantitative and well controlled data.

The control and characterisation of the polarisation of the light will also be an important asset for the science at the SARPES station. In systems where the spin texture is caused or influenced by spin-orbit coupling (SOC), the spin polarization of photoelectrons can be manipulated in three dimensions through selection of the light polarization (as demonstrated for example by studying topological insulators with highly polarized laser light [4]). For SOC systems the spin and orbital degrees of freedom are intrinsically coupled, thus any attempt to fully characterise the spin texture, for example by SARPES measurements, will require a well defined orbital selection. This can be achieved using pure polarisation states of the light, that are able to excite a given linear combination of orbitals. This is especially important when studying spin interference effects and when aiming at determining the degree of initial state spin polarisation. Although spin interference was described earlier [8], it is only by using the well-defined and variable polarisation of laser sources that the full implications have become clear [7, 6]. However, lasers have strong limitations in photon energy range and tunability and so the impact of this finding has remained limited. If a similar purity and variability of the light polarisation can be implemented at a synchrotron source, this will open up a whole new field of research. Besides the detailed characterisation of spin textures and degree of polarisation of quantum materials, it will also open up the pathway to imaging hidden order parameters and exotic quasiparticle interactions. Failing to providing controlled polarisation will result in following path of simple qualitative approaches, that will be inadequate for fully understanding SOC systems and limit the potential impact of the SARPES endstation Bloch.

6.3.2 6-axis manipulator

Due to a restricted budget, the SARPES endstation will begin operation offering only a 4-axis cryomanipulator. Although partially mitigated by the ability to perform small electronic tilt and polar adjustments, this still represents a serious limitation of the experimental capabilities of this endstation.

Today, much more so than when the A-branch was being procured, several high performance 6-axis cryomanipulators are available commercially from vendors such as CryoArc², Fermi³, HPM Precision⁴, ScientaOmicron⁵, Prevac⁶ and of course Specs⁷. Despite this wealth of options, the typical prices start at over 1.5MSEK (150 k€) and can reach twice that for very high performing models. Without a large infrastructure grant, this is infeasible.

Fortunately there is another option, which is to build a replica of the 'Geneva-Diamond' 6-axis manipulator that is deployed at the i05 ARPES endstation at Diamond Light Source. We are close to finalizing a legal agreement with Diamond Light Source and the University of Geneva that will allow us to purchase some of the specialized components from third party manufacturers and to fabricate the bulk of it internally in the MAX IV mechanical workshop. Particularly given that we already have the 4-axis stage and closed cycle cryostat, this will be something that can be completed using only the small upkeep grants awarded within MAX IV. Progress to date has been slowed by obtaining the legal agreement and by the lack of time of the main project responsible (C.P.) to drive the design modifications and coordinate with the MAX IV resource groups. Nonetheless, we remain optimistic that this project can be realized, in a time-frame that will permit us to offer it to SARPES users in 2023. In any case it is clear to us that replacing the 4-axis manipulator is mandatory for B-branch to

²<https://cryoarc.com>

³<http://en.fermi.com/>

⁴<https://www.omnivac.de>

⁵<https://scientaomicron.com>

⁶<https://www.prevac.eu>

⁷<https://www.specs-group.com>

deliver on its potential, and should the 'Geneva-Diamond' project fall through for whatever reason we will need to seek the necessary funding to obtain a commercial 6-axis manipulator.

6.3.3 Flexible sample environments

As mentioned in Section 2.3, the B-branch endstation design accommodates the possibility of exchanging manipulators in order to offer flexibility in the sample environment. In the following we provide a few examples of projects for adapted environments, some of which reflect clear expressions of interest from within our user community while others veer more towards speculation.

Strain One of the areas of growing interest among the user community is studying the effect of strain on electronic structure [11, 10]. These are of interest at Bloch specifically since a small light spot makes it possible to sample at well defined strains with minimal broadening even in the presence of a strain gradient. There have already been a few experiments at Bloch using passive strain sample holders, where the strain changes with temperature. Active approaches based on piezoelectric actuators would bring several advantages, but require specialized sample manipulators with multiple electrical contacts and potentially larger sample spaces. As part of a project led by an external user group, we will test such a manipulator and associated active strain cell on the SARPES endstation at Bloch, benefiting from the possibility for rapid exchange of the manipulator and with a view to adapt such capabilities for general users in the future.

Currents and applied fields Another interesting direction we have seen user proposals take is measuring band structure while passing a small current through the sample, usually to drive a phase transition. Here again a small spot size is crucial as the energy broadening is proportional to the magnitude of the potential gradient within the light spot. At present such an experiment can be conducted in a limited way at the A-branch endstation, where current can be passed through a sample at a specific azimuthal orientation. Related to this, we have also observed with interest the growing number of reports of successful gating schemes in ARPES experiments [9, 3, 5]. We believe that a manipulator customized towards combining ARPES with transport or gating would possess a great deal of potential.

Micro-positioning manipulators One of the consequences of the $10\mu\text{m} \times 10\mu\text{m}$ beam size at Bloch is that the investigations and techniques begin to show some overlap with nanoARPES facilities. Specifically we have watched the increasing adoption and value of performing spatially-resolved ARPES maps. Unlike the nanoARPES facilities however, Bloch was not designed with rapid and efficient sample scanning in mind - neither the acquisition software (SES) nor the large manipulator lend themselves to this application. For some applications then it may be worth investigating. We therefore consider the potential value of a specialized manipulator incorporating piezoelectric-based translation stages. One additional benefit here would be in the form of experience gained for a potential future development of a dedicated submicron ARPES endstation, discussed in the following section.

6.3.4 Submicron/nanoARPES

In the past few years the publications emerging involving submicron/nano-ARPES have clearly demonstrated both the value of this technique but also that there is considerable potential here, with the number of applications only growing as the technique matures. One example that is of particular interest to the Swedish user community is the fast emerging field of van der Waals heterostructures, where samples lengthscales range from a few hundred nanometers to a few micrometers.

Already a few synchrotron facilities provide this capability, e. g. Maestro at ALS, I05 at DLS, Antares at Soleil, Spectromicroscopy at Elettra and the upcoming AU-SGM3 at Astrid-2. Apart from benefiting groups who use the ARPES technique for fundamental studies, the possibility of

using sub-micron beams will attract researchers interested in device oriented applications, where the electronic structure of the functional parts of the device can be mapped with high lateral resolution or for *operando* electronic structure studies of proof-of-principle quantum devices. It is clear from the investment in quantum technologies both in Sweden and internationally that this is a fast emerging field.

The first goal we are interested in pursuing at Bloch is to achieve a sub-micron spot size through the implementation of capillary optics and/or zone plates, to prove that nanoARPES is within reach at this beamline. A 'Expression of Interest' in this direction has been prepared as a collaboration with KTH University as input for the [MAX IV research roadmap](#). A second, more challenging step, will be the design and implementation of a sample stage with stability and reproducibility to match the desired spatial resolution. This is, however, far from our immediate horizon. One aspect to carefully consider in future, if one plans to implement nanoARPES at Bloch, is whether the energy range for which Bloch provides optimal performance (10-200 eV) is suited to the envisioned applications. For sufficiently clean and 2D or surface-dominated systems this is true, but for example *operando* device applications would likely benefit from operating in the soft X-ray regime (200-2000 eV) where the electron escape depth is larger. This could be implemented at Veritas beamline, where the high brilliance of the 3 GeV ring of MAX IV Laboratory is a key ingredient for the production of extremely focused X-ray beams.

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