HZB Helmholtz Zentrum Berlin

Experimental Facilities at BESSY II and BER II

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Thomas Frederking

Preface

Excellent science needs excellent facilities. One central mission of the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) is to provide such excellent opportunities. Operating two state-of–the-art large-scale facilities, the third generation synchrotron source BESSY II and the neutron research facility BER II, HZB offers a broad range of instruments, beamlines, analytical facilities and laboratories which create unique opportunities for leading-edge research in a wide range of scientific areas.

The BESSY II synchrotron radiation source, a 1.7 GeV storage ring dedicated to the VUV and soft X-ray photon spectrum, serves an international user community. The source and the instrument suite are very versatile and provide photons at a high average brilliance, which allows – at repetition rates up to 500 MHz – for high resolution energy (~meV), spatial (10 nm), and temporal (sub-picosecond) control, as well as polarisation control. The access to very low (<0.01 eV) and high (>10 keV) photon energies facilitates dedicated experiments in the areas of materials and energy research, catalysis, chemical reactions and structural biology. A number of beamlines are operated with collaborative partners such as the Max Planck Society (MPG), the German Federal Institute for Materials Research and Testing (BAM), the German national metrology institute Physikalisch-Technische Bundesanstalt (PTB) and many German universities. MPG, for example, will operate the CAT Laboratory (Catalysis Research for a Sustainable Energy Supply) within the new Energy Materials In-situ Laboratory EMIL, where scientists will investigate catalytic and photocatalytic processes.

The profile of neutron scattering research at the BER II medium-flux neutron source is characterised by a recently upgraded and optimised instrument suite for neutron scattering and imaging with thermal as well as cold neutrons. Sample environments for complex neutron experiments under extreme conditions such as high magnetic fields and extremely low temperatures generate special research opportunities. The new High Field Magnet facility currently being installed and set to go into operation in 2015, combines neutron scattering with the highest field strengths to explore new science.

In addition, with the LabCluster, HZB offers its users a number of state-of-the-art on-site laboratories for sample synthesis and characterisation. All these facilities are designed to serve researchers from universities, foreign research institutions and industry.

The combination of the multi-user radiation sources and associated laboratories provides scientists from a wide variety of research areas with access to a broad range of instruments and complementary methods. HZB strongly encourages scientists to take advantage of this unique opportunity to exploit both sources within one centre. A unified, peer-reviewed proposal system opens up access to both sources and the LabCluster to users worldwide.

This booklet gives a comprehensive overview of the entire portfolio of instruments and laboratory facilities on offer to users at the large-scale facilities operated by HZB. More information is available on the HZB website. We hope this will help you to choose the best instruments for the best science, and look forward to receiving your proposals.

Prof. Dr Anke Kaysser-Pyzalla
Scientific Director

Thomas Frederking
Administrative Director

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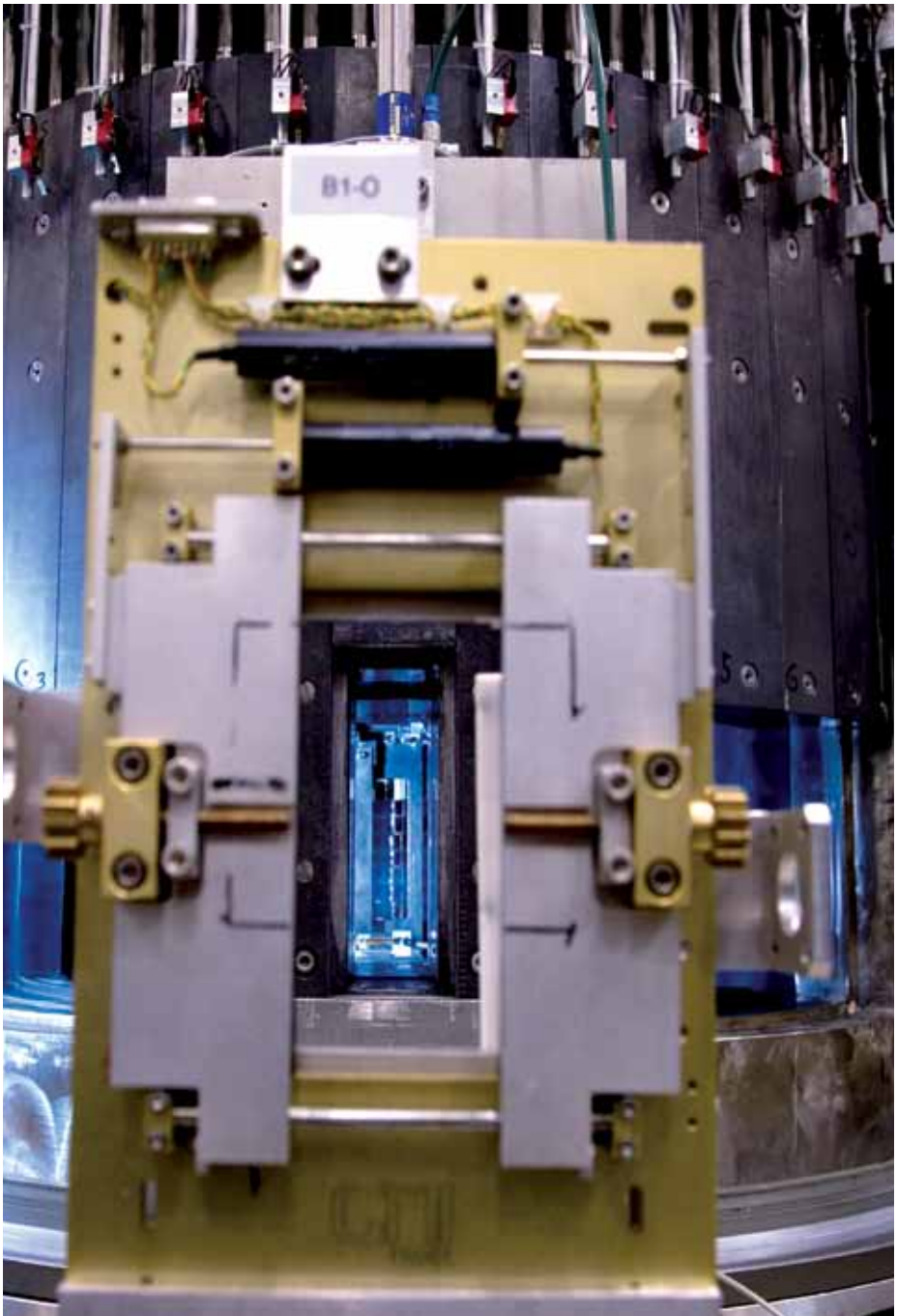

Synchrotron Facility BESSY II

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

FIXED STATIONS BESSY II

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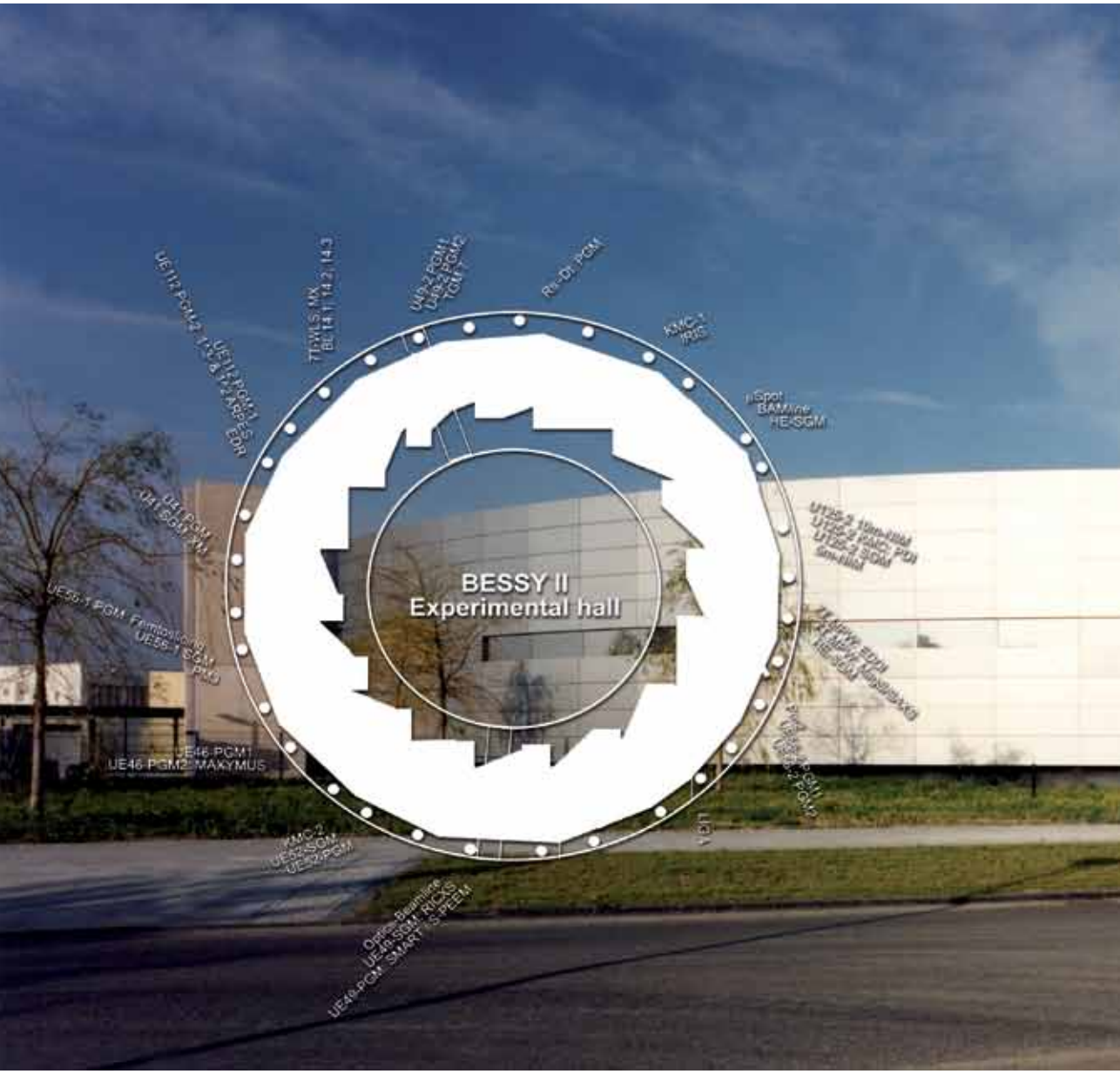

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PROJECTS

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Photon source BESSY II

The storage ring BESSY II in Adlershof is at present the only third generation synchrotron radiation source in Germany. BESSY II emits extremely brilliant photon pulses ranging from the long wave terahertz region to hard X-rays. Users can choose the energy range and the polarisation of the radiation. The forty six beam holes at the undulator, wiggler, and dipole sources offer users a many-faceted mix of beam holes and measuring sites with outstanding energy resolution. The combination of brilliance and photon pulses makes BESSY II the ideal microscope for space and time, allowing resolutions down to femtoseconds and picometres.

An important role is played by the scientists at the HZB, but also the institutional users like the Max Planck Society, the Federal Institute for Materials Research and Testing, and collaborating research groups. Consequently, as a result of the activities by the Physical Technical Institute PTB, BESSY II is the European radiation standard for the calibration of light sources and detectors.

BESSY II employs an electron gun to generate a 70 kV electron beam. Before injection in the main storage-ring the beam is accelerated over a microtron and a synchrotron to its final energy of 1.7 GeV. The accelerating process

takes 50 ms and can be repeated with a repetition rate of 10 Hz. The total current in the storage ring of 300 mA can be obtained by successive injection of electrons, accelerated in multiple accelerating cycles.

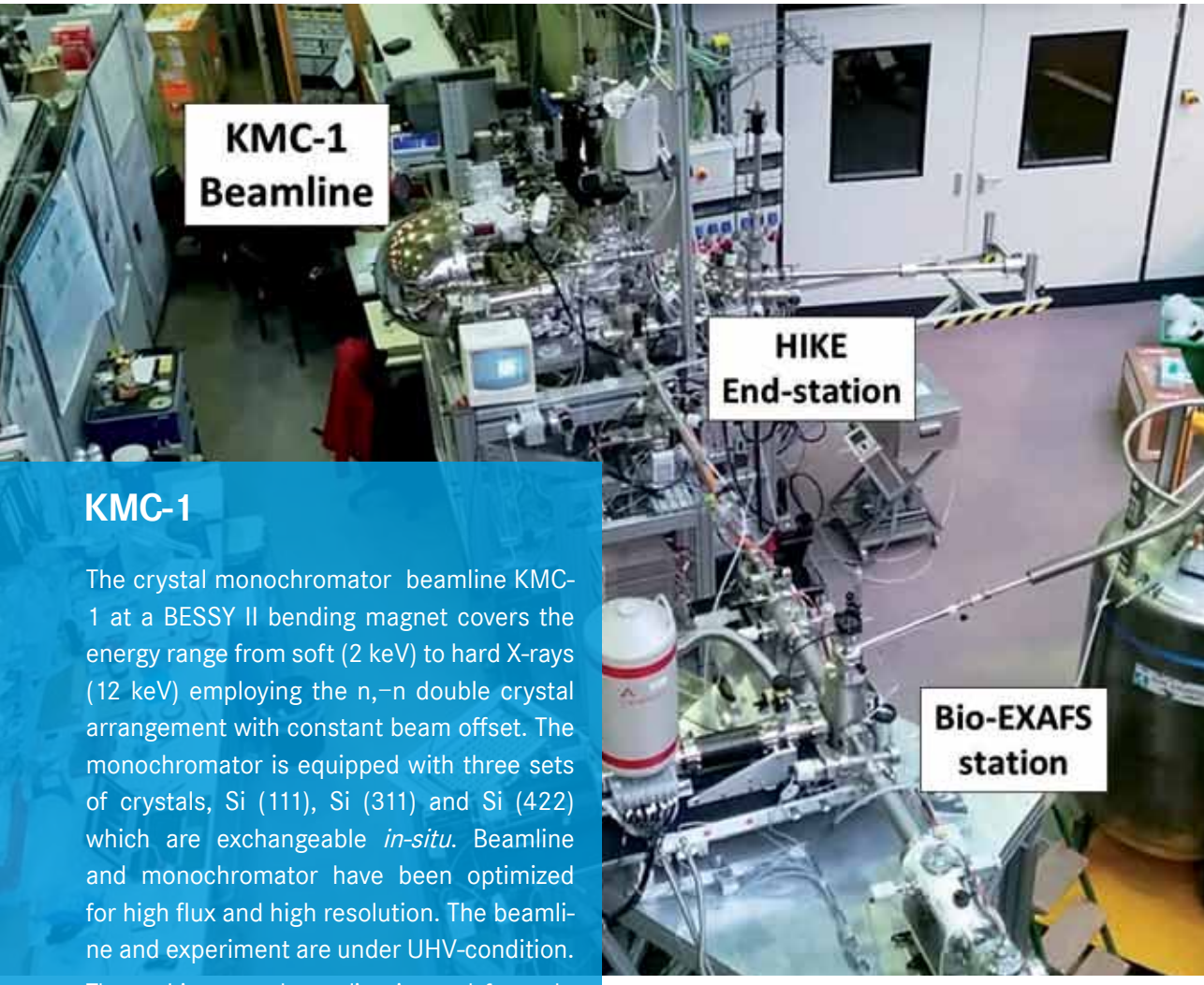
The storage ring BESSY II is extremely flexible by using low-alpha operation mode and superconducting insertion devices. Starting in the THz region the energy range spans more than eight orders of magnitude and reaches into the hard X-ray regime delivering synchrotron radiation to some 50 experimental stations. Of the 16 straight sections 14 are equipped with insertion devices the most challenging being the new UE-112, a 7T multipole wiggler, and the femtoslicing assembly.

Storage ring specifications

- **Year:** 1998 BESSY II operation begins
- **Merger:** 2009 merger of BESSY GmbH and Hahn Meitner Institute into the Helmholtz Center for Materials and Energy GmbH
- **Storage ring:** circumference 240 m
- **Deflecting magnets:** 32
- **Pulse duration:** approximately 20 picoseconds
- **Electron energy:** 1.7 GeV
- **Nominal beam current:** 300 mA
- **Energy range of emitted radiation:** from coherent THz radiation up to 150 keV
- **Total number of beamlines or end stations:** 43

BESSY II

Beamlines Open Port



KMC-1

The crystal monochromator beamline KMC-1 at a BESSY II bending magnet covers the energy range from soft (2 keV) to hard X-rays (12 keV) employing the n,–n double crystal arrangement with constant beam offset. The monochromator is equipped with three sets of crystals, Si (111), Si (311) and Si (422) which are exchangeable *in-situ*. Beamline and monochromator have been optimized for high flux and high resolution. The beamline and experiment are under UHV-condition.

The multipurpose beam line is used for techniques such as hard X-ray high kinetic photoelectron spectroscopy (HIKE or HAXPES), (Bio)-EXAFS, NEXAFS, absorption, reflection and fluorescence spectroscopy. Due to the windowless UHV-setup the k-edges of the technologically and biologically important elements such as Si, P, and S are accessible. Photon flux in the 10^{11}–10^{12} photons/s range and beamline resolving powers of more than 100.000 have been measured at selected energies. Thus, HAXPES with a total instrumental resolution of about 150 meV is possible at selected energies.

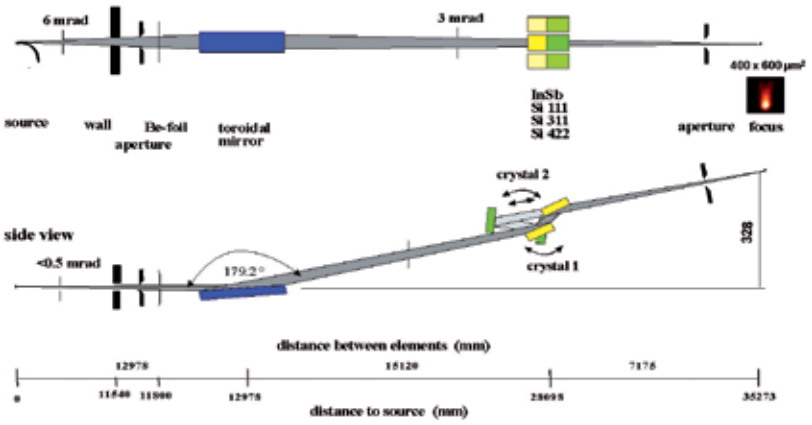
The beamline is not permanently equipped with a particular experimental station but rather varying user experiments are connected to it according to the beamtime schedule. Based on the allocated beamtime the HIKE end-station is the main user of the KMC-1 beamline.

Instrument application

- HIKE (High Kinetic Energy Photoelectron Spectroscopy) or HAXPES (Hard X-ray Photoelectron Spectroscopy)
- EXAFS, NEXAFS, XANES
- Diffractometry, Reflectometry

Instrument data

Location	3.1
Source	D11
Monochromator	KMC-1
Energy range	2 – 12 keV
Energy resolution	1000 at 4 keV
Flux	10^{11} at 4 keV
Polarisation	Horizontal
Divergence horizontal	3 mrad
Divergence vertical	0.2 mrad
Focus size (hor. x vert.)	0.4 x 0.6 mm
Distance Focus/last valve	670 mm
Height Focus/floor level	1728 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Franz Schäfers, franz.schaefers@helmholtz-berlin.de Dr. Mihaela Gorgoi, mihaela.gorgoi@helmholtz-berlin.de Marcel Mertin, marcel.mertin@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

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[2] Gerlach, D. *et al.*: The silicon/zinc oxide interface in amorphous silicon-based thin-film solar cells: Understanding an empirically optimized contact, Appl. Phys. Lett., 103 (2013), 023903.

[3] Slooten, E. *et al.*: Hard X-ray photoemission and density functional theory study of the internal electric field in $SrTiO_3/LaAlO_3$ oxide heterostructures, Phys. Rev. B, 87 (2013), 085128.

[4] Kundu, S. *et al.*: A High-Valent Heterobimetallic [Cu-III(mu-O)(2)Ni-III](2+) Core with Nucleophilic Oxo Groups, Angew. Chem. Int. Ed., 52 (2013), 5622-5626.

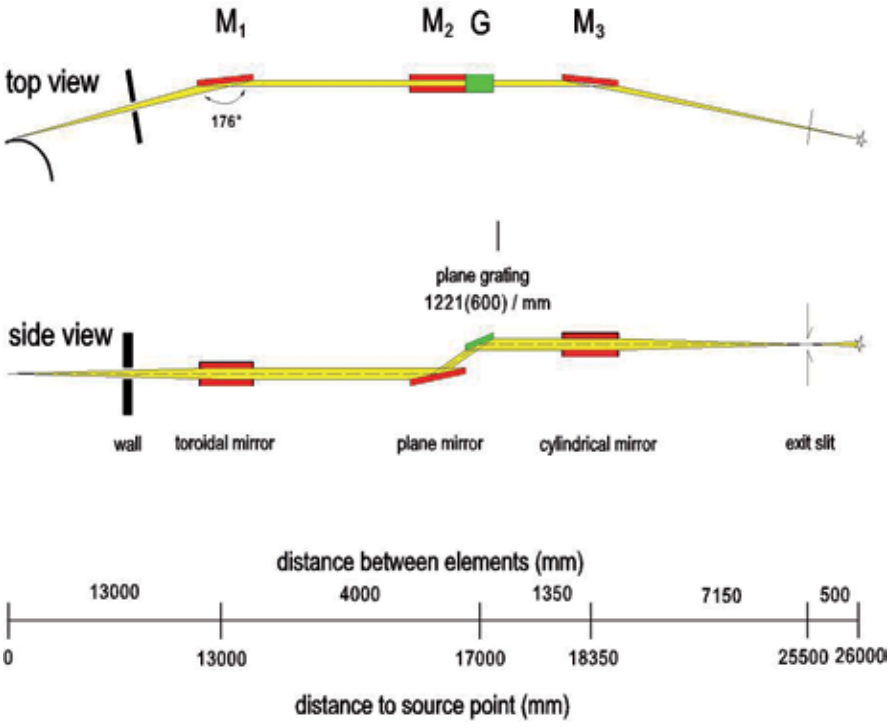
[5] Schäfers, F. *et al.*: KMC-1: a High Resolution and High Flux Soft x-Ray Beamline at BESSY, Rev. Sci. Instrum. 78 (2007), 123102.

KMC-1 - Reference guide for latest publications

PM3

PM3 is designed to deliver synchrotron radiation of variable polarization (linear and left- or right-handed elliptical), easily tuneable over a wide range of photon energies. Operating in the soft X-ray range, the major part of beamtime is dedicated to the investigation of magnetic materials using magnetic circular dichroism (XMCD) techniques. It is an “open port” beamline meaning that it is not equipped with a permanent experimental station. Rather, varying user experiments are connected to the PM3 beamline according to the beamtime schedule. At BESSY II PM3 has been installed in 2001.

The accessible photon energies range from about 30 to 2000 eV. The energy resolution of 32 000 @ 64 eV is the best reported for any SX700 type monochromator so far. A signal-to-noise ratio close to the shot noise level, fast “on-the-fly” scanning and horizontal beam position control make PM3 one of the most productive dipole beamlines at BESSY II.



Optical Layout

Instrument data

Location	12.2
Source	D111
Monochromator	PM3
Energy range	20 - 1900 eV
Energy resolution	32000 at 64 eV
Flux	10^9 - 10^{10}
Polarisation	• Horizontal • Circular
Divergence horizontal	1.5 mrad
Divergence vertical	1 mrad
Focus size (hor. x vert.)	300
Distance Focus/last valve	500 mm
Height Focus/floor level	1432 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Torsten Kachel, torsten.kachel@helmholtz-berlin.de Dr. Brian O' Cinneide, brian.ocinneide@helmholtz-berlin.de

Instrument application

- Sub-Monolayers to Multilayers (inorganic or organic)
- Liquids
- Ferrimagnets
- Exchange Bias systems
- Multiferoics
- Magnetic Nanoparticles

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

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[2] Antoniak, C. *et al.*: A guideline for atomistic design and understanding of ultrahard nanomagnets, Nature Communications 2 (2011), 528.

[3] Valencia, S. *et al.*: Interface-induced Room-Temperature Multiferroicity in $BaTiO_3$, Nature Materials 10 (2011), 753-758.

[4] Radu, F. *et al.*: Perpendicular Exchange Bias in Ferrimagnetic Spin Valves, Nature Communications 3 (2012), 715.

[5] Luo, Y. *et al.*: Imine Derivatives on Au(111) for the Formation of Aromatic Mixed Self-Assembled Monolayers, Langmuir 28 (2012), 358-366.

[6] Manzke, A. *et al.*: Formation of Highly Ordered Alloy Nanoparticles Based on Precursor-Filled Latex Spheres, Chem. Mater. 24 (2013), 1048.

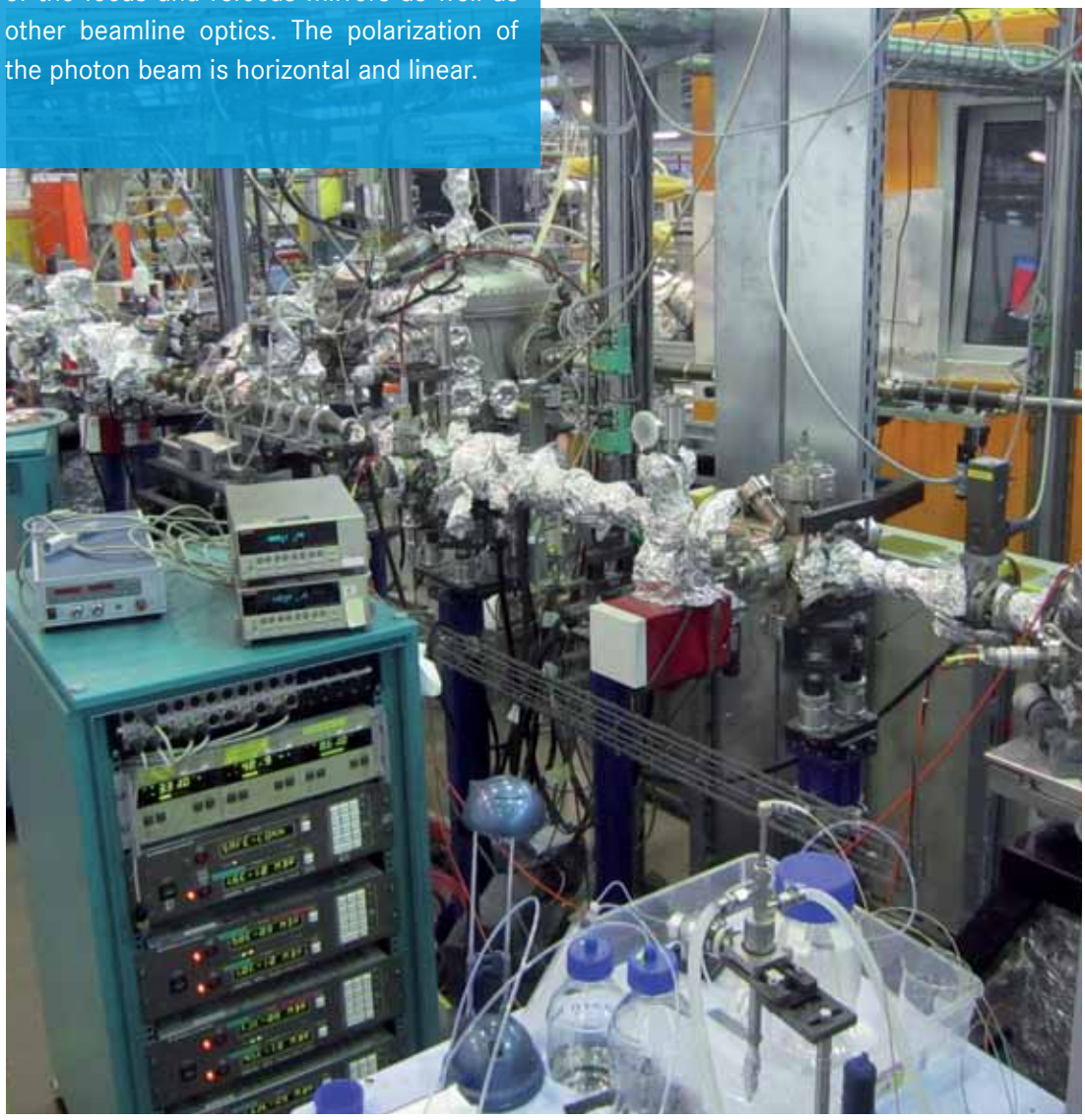
PM3 - Reference guide for latest publications

U41 PGM

U41-PGM is a microfocus beamline with flexible end-stations. It provides high photon flux (~ 10^{13} photon/sec) and small focal size (36 µm x 12 µm, hor. x vert.) in soft X-ray range. The high flux comes from U41 undulator which delivers the highest brilliance among Bessy's undulators. The microfocus benefits from the low-ß section and the fine-tuning of the focus and refocus mirrors as well as other beamline optics. The polarization of the photon beam is horizontal and linear.

Instrument application

- Low concentration samples which require high flux (multi-bunch mode)
- Diluted liquid solution, and low concentration solids
- Liquid flow cell (with membrane absorbing transimitted photon)
- Small size samples which require small focus (multi-bunch mode)
- Liquid micro-jet (diameter of 20 µm or less)
- Samples that require high spatial resolution
- Pump-probe measurement at single-bunch mode



Instrument data

Location	13.2
Source	U41
Monochromator	PGM
Energy range	170 - 1800 eV
Energy resolution	> 2000
Flux	10^{13}
Polarisation	Horizontal
Divergence horizontal	1.2 mrad
Divergence vertical	0.5 - 2.5 mrad
Focus size (hor. x vert.)	The best is 36 µm x 12 µm (FWHM) at exit slit 20 µm and Cff 0.1. It is of bigger size for Cff 0.65.
Distance Focus/last valve	504 mm
Height Focus/floor level	1376 mm
Free photon beam available	Yes
Fixed end station	No
Premonochromator optics	M1: toroidal mirror, horizontal deflection, 2Θ=176°, gold coated, water cooled, vertical collimation, horizontal focusing onto exit slit
Monochromator	Principle: plane grating monochromator with collimated light, operated at negative diffraction order (cff < 1) Optical components: G1: plane gratings, 600 l/mm, blaze 0.8°, vertical deflection, 2Θ=169-175°, gold coated, water cooled M2: plane mirror, vertical deflection, 2Θ=169-175°, gold coated, water cooled
Focusing mirror	M3: cylindrical mirror, horizontal deflection, 2Θ=176°, gold coated, vertical focusing onto exit slit
Exit slit	Slit settings: 20/40/100/200/500/2000/3000 µm ± 200 mm translation
Postmonochromator optics	M4: toroidal mirror, horizontal deflection, 2Θ=176°, gold coated, vertical and horizontal demagnification of exit slit into sample area
Instrument responsible	Jie Xiao, jie.xiao@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Follath, R., Senf, F.: New plane-grating monochromators for third generation synchrotron radiation light sources, Nucl. Instr. Meth. vol. A390 (1997), 388-394.

[2] Weiß, M.R. *et al.*: Comparative monochromator studies for a soft X-ray microfocus beamline for BESSY-II, J. Electr. Spectrosc. Relat. Phenom. vol. 101-103 (1999), 1003-1012.

U41 PGM - Reference guide for latest publications

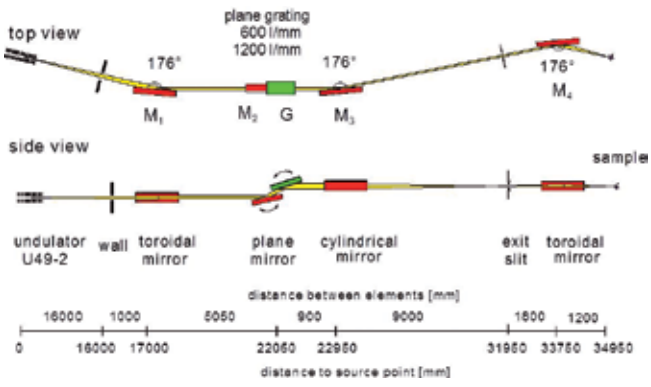
Synchrotron Facility BESSY II

U49-2 PGM-1

The plane grating monochromator U49/2 PGM1 delivers soft X-ray undulator radiation of linear polarization between 84 and about 1500 eV. High photon flux combined with high stability and a comparatively small spot size allow for “photon hungry” experiments like *e.g.* coincidence methods, photo-excitation on liquid jets or clusters. Experiments have a strong focus on surface chemistry and surface physics but also serve selected topics in molecular and atomic science. The high demand of these radiation properties is visible by the overbooking in beam time requests and the number and quality of high impact publications by external and in-house users.

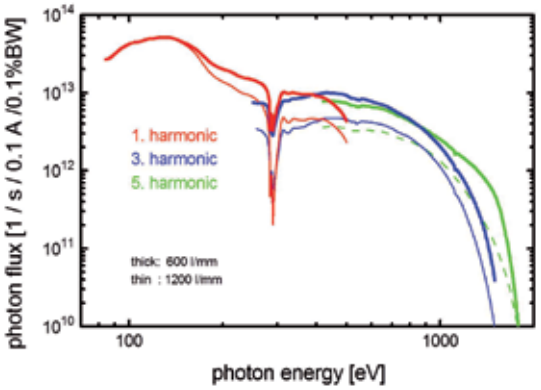
Instrument application

- Material Science
- Molecular Physics/Dynamics
- Surface Science
- Soft X-ray Microscopy
- Liquids



Instrument data

Location	16.2
Source	U49-2
Monochromator	PGM-1
Energy range	85 - 1600 eV
Energy resolution	25000 (85-500 eV) / 15000 (500-1500 eV) (standard grating)
Flux	10^{13} ph/s (85-500 eV) 10^{12} ph/s (500-1500 eV) (standard grating)
Polarisation	Horizontal
Divergence horizontal	2 mrad
Divergence vertical	2 mrad
Focus size (hor. x vert.)	80 µm x 22 µm
Distance Focus/last valve	959 mm
Height Focus/floor level	1417 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Torsten Kachel, torsten.kachel@helmholtz-berlin.de Prof. Dr. Gregor Schiwietz, schiwietz@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Gleichweit, C. *et al.*: Dehydrogenation of Dodecahydro-N-ethylcarbazole on Pt(111), ChemSusChem 6 (2013), 974-977.

[2] Papp, C. *et al.*: In situ high-resolution X-ray photoelectron spectroscopy – Fundamental insights in surface reactions, Surface Science Reports 68 (2013), 446.

[3] Ortel, E. *et al.*: Mesoporous and Hierarchical Porous Pd/TiO_2 Catalytic Coatings, Chem. Mater. 24 (2012), 3828-3838.

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U49-2 PGM-1 - Reference guide for latest publications

U125-2 NIM

Normal incidence monochromators (NIM) are typically used in synchrotron beamlines which are dedicated to experiments operating in an energy range of about 4 to 35 eV only. The decisive advantages of this type of monochromator design are that only small aberration errors occur and highest resolution can be easily achieved with it.

The 10m-NIM beamline (Reichardt *et al.* 2001) was designed for the undulator U125-2 (Bahrdt *et al.* 2001) and is based on the so called off-Rowland circle mounting design (Samson 1967). This implies that the grating has to be rotated and slightly translated in order to get the highest resolution and a small spot size in the experiment.


Overview


10m-NIM


Experiment Platform

Instrument application

At this beamline the users care for their own experimental setup which fits to their application. Typical user's applications and experimental methods are absorption spectroscopy, fluorescence spectroscopy, photoelectron spectroscopy, photoionization of molecules and clusters, spectroscopic ellipsometry.

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

Instrument data

Location	5.1
Source	U125-2
Monochromator	10m-NIM
Energy range	6(4) - 40 eV
Energy resolution	E/dE = 85000 @ d = 1200 l/mm, 2nd order, 10 µm slits
Flux	10^{12} @ 21.75 eV [photons/s/0.1A/0.1%BW]
Polarization	Horizontal
Divergence horizontal	5.5 mrad
Divergence vertical	12 mrad
Focus size (hor. x vert.)	200 x 350 μm^2
Distance Focus/last valve	1190 mm
Height Focus/floor level	1750 mm (1400 mm with concrete experiment platform)
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Peter Baumgärtel, peter.baumgaertel@helmholtz-berlin.de Ingo Packe, ingo.packe@helmholtz-berlin.de

References / Latest publications

[1] Reichardt, G. *et al.*: A 10m-normal incidence monochromator at the quasi-periodic undulator U125-2 at BESSY II, In NUCL INSTRUM METH A 467 (2001), 462-465.

[2] Bahrdt, J. *et al.*: A quasi-periodic hybrid undulator at BESSY II. In NUCL INSTRUM METH A 467-468 (2001), 130-133.

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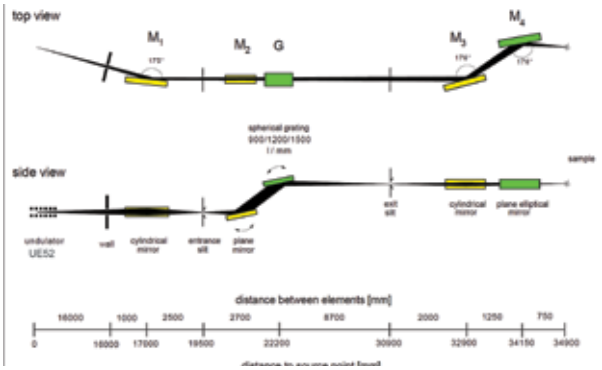
U125-2 NIM - Reference guide for latest publications

UE52 SGM

Soft X-ray beamline for flexible end stations with variable polarization covering the range of 90 - 1500 eV with an X-ray spot size of approximately 60 µm (horizontal). The polarization can be freely chosen between linear (any orientation) and circular.

Instrument application

- Magnetism and Magnetization dynamics
- Holography, coherent diffractive imaging
- Self-assembled monolayers, photoswitches
- Single-molecule magnets (surfaces)
- Correlated systems, superconductivity
- Nanoparticles, aerosols, clusters
- Atomic and molecular physics (gas phase)



Instrument data

Location	10.2
Source	UE52
Monochromator	SGM
Energy range	90 - 1500 eV
Energy resolution	> 4000
Flux	> 10^{12}
Polarization	Variable
Divergence horizontal	6 mrad
Divergence vertical	1 mrad
Focus size (hor. x vert.)	60 µm (hor)
Distance Focus/last valve	530 mm
Height Focus/floor level	1417 mm
Free photon beam available	Yes
Fixed end station	No
Premonochromator optics	M1: cylindrical mirror, horizontal deflection, 2Θ=175°, gold coated, water cooled, vertical demagnification (17:2.5) of source on entrance slit
Entrance slit	Slit setting: 0-2000 µm, water cooling, insolated blades for vertical beam position sensing, on line laser diffraction slit width monitor
Monochromator	Principle: variable deflection angle, focused spherical grating monochromator Optical components: M2: plane mirror, vertical deflection, 2Θ=169-175°, gold coated, water cooled G1-3: spherical gratings, vertical deflection, 2Θ=169-175°, gold coated, water cooled
Exit slit	Slit setting= 0-2000 µm, ±200 mm translation, on line laser diffraction slitwidth monitor
Postmonochromator optics	M3: cylindrical mirror, horizontal deflection, 2Θ=176°, gold coated, vertical demagnification (1:1) of exit slit M4: plane elliptical mirror, horizontal deflection, 2Θ=176°, gold coated, horizontal demagnification of source
Instrument responsible	Priv.-Doz. Dr. Philippe Wernet, wernet@helmholtz-berlin.de Dr. Wilson Quevedo, wilson.quevedo@helmholtz-berlin.de Dr. Piter Sybren Miedema, piter.miedema@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Senf, F. *et al.*: Performance of the first undulator beamline U49-1-SGM at BESSY II, Nucl. Instrum. Meth. A 467-468 (2001), 474-478.

[2] Godehusen, K. *et al.*: Electron-correlation effects in the angular distribution of photoelectrons from Kr investigated by rotating the polarization axis of undulator radiation, Phys. Rev. A 68 (2003), 012711.

UE52 SGM - Reference guide for latest publications

UE56-1 ZPM

The ZPM-monochromator was particularly designed and commissioned according to user requirements to support optical-pump- soft X-ray probe experiments at the FemtoSpex facility at the UE56-1. Owing to the principles of generating 100 fs X-ray pulses from a storage ring [1] one needs optics of highest possible transmission up to 21%. A successful approach has been a single element monochromator based on Reflection Zone Plates [2]. The current design as depicted in Figure 1 (right) consists of 9 lenses that enable a working range from 410 to 1333 eV at moderate spectral resolutions of E/ΔE= 500 or, in one case E/ΔE = 2000, at 713 eV. The optics is tailored to minimize pulse elongations to 30 fs preserving the polarization properties of the elliptical light from the undulator.

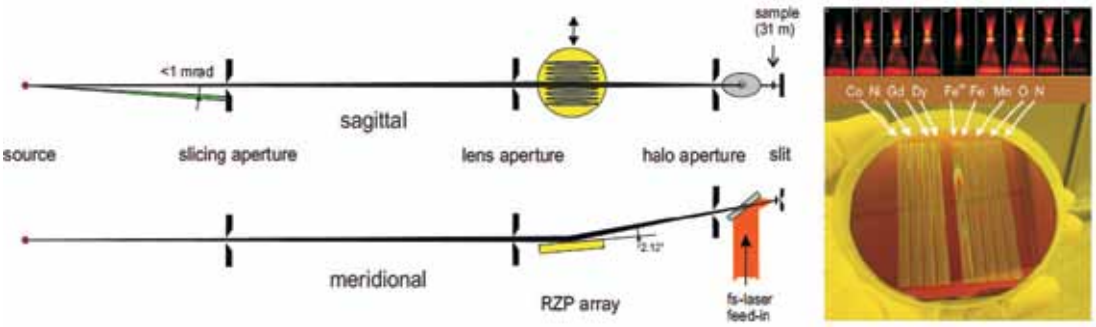


Figure 1: Optical layout (left) of the high transmission (T ~ 0.2) ZPM beamline after the upgrade in 2012. In order to select a certain lens (image) and energy range, the optical element (RZP array, yellow) is moved perpendicular to the optical axis driven by a stepping motor. A special laser feed-in (orange) is an inherent part of the approach enabling pump-probe experiments with variable pump wavelength from UV to FIR at large numerical aperture. The red images above the right picture show the intensity distributions in the focus after each lens [2].

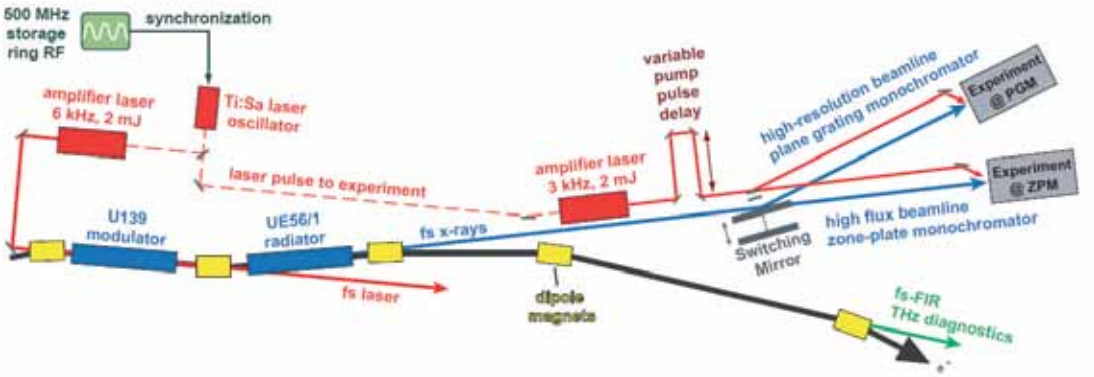


Figure 2: Schematic layout of the full optical pump-soft-X-ray probe setup at the FemtoSpeX facility after the laser (red boxes) and repetition rate upgrade. The horizontal dimension of the entire setup is ca. 50 m. Synchronized to the 500 MHz master-oscillator driving the rf-cavities of the ring, a Ti:Sa oscillator seeds the two regenerative amplifiers that are located in different laser hutches. Both the X-ray beam (blue) and the laser beam (red) travel a similar pathway (in-vacuum) to the experiment, while part of it is bridged by the transversely actively stabilized oscillator beam (dashed red line). As a monochromator, either the high resolution Plane Grating Monochromator (PGM) or the high flux Zone Plate Monochromator (ZPM) can be selected by setting a switching mirror to the corresponding position.

Instrument data

Location	12.2
Source	UE56-1 slicing
Monochromator	Reflection Zone Plate Arrray (RZPA)
Energy range	410 - 1330 eV
Energy resolution	500/2000
Flux	$1 \cdot 10^6$ ph/sec/0.1%BW@6kHz (100 fs pulses)
Polarisation	Variable
Divergence horizontal	0.2 mrad
Divergence vertical	0.1 mrad
Focus size (hor. x vert.)	140 µm x 40 µm (slit)
Distance Focus/last valve	800 mm
Height Focus/floor level	1763 mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Karsten Holldack, karsten.holldack@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Holldack, K. et al., FemtoSpeX - A versatile optical pump - X-ray probe facility with 100 fs X-ray pulses of variable polarization, Journal of Synchrotron Rad. 21 (2014), doi:10.1107/S1600577514012247.

[2] Brzhezinskaya, M, *et al.*: A novel monochromator for experiments with ultrashort X-ray pulses, Journal of Synchrotron Radiation 20 (2013), 522-530.

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[4] Boeglin, C. *et al.*: Distinguishing the ultrafast dynamics of spin and orbital moments in solids, Nature 465 (2010), 458-462.

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[7] Eschenlohr, A. *et al.*: Ultrafast spin transport as key to femtosecond demagnetization, Nature Materials 12 (2013), 332-336.

[8] Bergerard, N. *et al.*: Ultrafast angular momentum transfer in multisublattice ferrimagnets, Nature Communications 5 (2014), 3466.

Instrument application

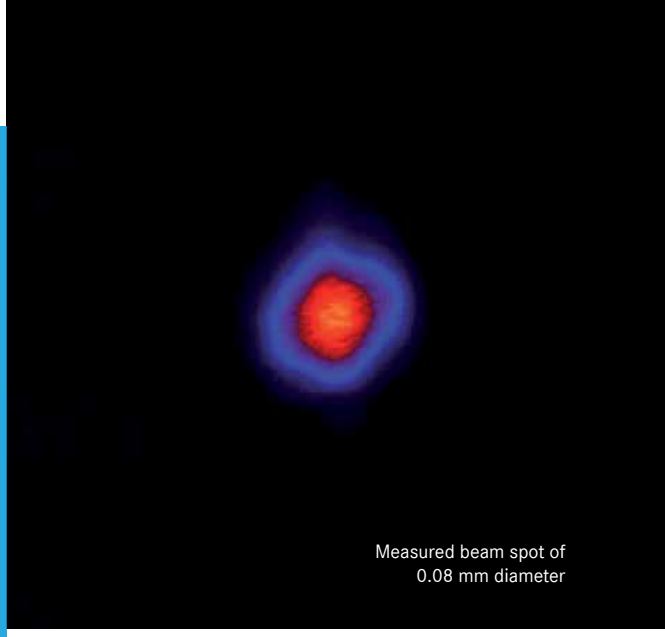
The temporal evolution of physical phenomena on fs-timescales is still widely uncharted territory and the mechanisms underlying phase transitions in solids and magnetization reversal on these timescales are still under debate. FemtoSpeX experiments at the ZPM can answer these questions [3-8]. Dedicated endstations that cover ultrafast magnetism experiments based on time-resolved XMCD have therefore been either been upgraded or, in case of time-resolved resonant soft X-ray diffraction (RSXRD) and reflection, newly constructed and adapted to Femtoslicing-requirements. Experiments at low temperatures down to 6 K and magnetic fields up to 0.5 Tesla are supported. The ZPM-monochromator as the main workhorse at the FemtoSpeX facility is now operated as a (shared) 24 h user facility enabling a new class of experiments in ultrafast magnetism and in the field of transient phenomena and phase transitions in solids.

UE56-1 ZPM - Reference guide for latest publications

UE112 PGM-1

UE112_PGM-1 is a low-energy high-flux beamline, providing X-rays of variable (linear and elliptical) polarization at high energy resolution. This is accomplished through a modern APPLE-II-type undulator and a plane-grating monochromator (PGM) in the beamline. The X-ray beam is focused into a small spot of a diameter of about 80 µm nearly without indications of a halo (see figure with measured beam intensity distribution). The focal distance from the last beamline valve is about 1 m and the usable target area is large enough to enable the installation of relatively large experimental setups. Thus, the beamline includes no fixed end station and it is optimized for variable modes of operation using very different internal and external experiment chambers (typically these are end stations). Some selected examples for such systems are:

- **PHOENEXS** – a (Spin Resolved) Photoemission and Near Edge X-ray Station, operated by HZB.
- **ArTOF** – various Angle-Resolved Time-of-Flight systems featuring high resolution and large detection solid-angle, operated by groups of Uppsala University and HZB.
- **COLTRIMS** – a system for Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) for electron/ion coincidences in the gas phase, operated by the group of R. Dörner, Goethe- Universität Frankfurt.
- **FlexRIXS** – a soft X-ray monochromator, for RIXS (Resonant Inelastic X-ray Scattering) investigations of fluid and solid-state target, operated by HZB.



Measured beam spot of 0.08 mm diameter

Detailed instrument description

The optical layout of the beamline (all values in the subsequent schema are design parameters, dimensions given in mm). M_1 is a toroidal mirror which collimates the light in the horizontal and vertical directions. The plane mirror M_2 is used to vary the deviation angle at the plane grating G. Vertically, the diffracted light is focused onto the exit slit S by the cylindrical mirror M_3. The subsequent refocusing is performed by the mirrors M_4 and M_5 in the vertical and horizontal directions, respectively. For actual measured values of the focus position (asterisk), look at the instrument-data table further below.

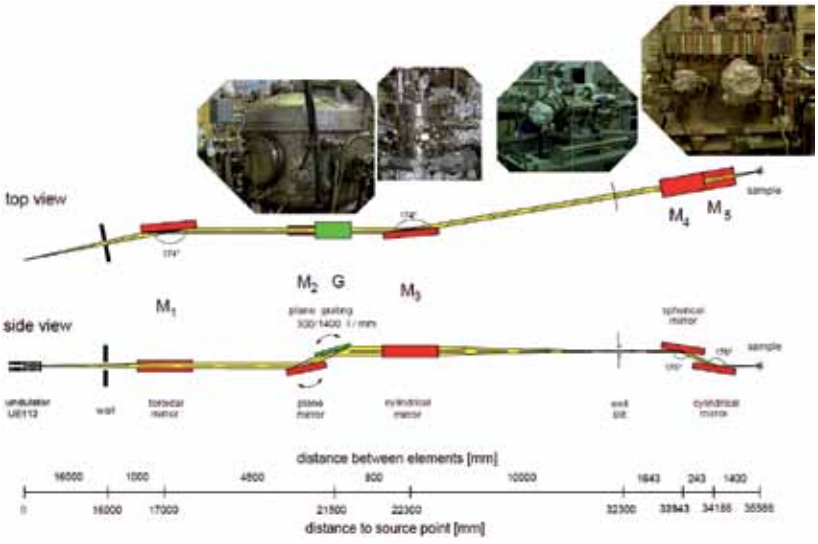
References

[1] Follath, R., Senf, F.: New plane-grating monochromators for third generation synchrotron radiation light sources, Nucl. Instrum. and Meth. A390 (1997), 388-394.

[2] Follath, R., Senf, F., Gudat, W.: Plane-grating monochromator at BESSY II using collimated light, J. Synchrotron Rad. 5 (1998), 769-771.

Instrument data

Location	14.2
Source	UE112
Monochromator	PGM
Energy range	17 – 690 eV; for extreme values (<50 eV or >400 eV) please contact the beamline crew in advance
Energy resolution	30000 (17-150 eV) > 20000 (150-350 eV) (standard grating)
Flux	> 10^{12} ph/s (20-280 eV) > 3 · 10^{13} ph/s (50-150 eV) (standard grating)
Polarization	Variable
Divergence horizontal	1.4 @ 63.5 eV mrad
Divergence vertical	0.6 @ 63.5 eV mrad
Focus size (hor. X vert.)	Optimum: ca. 0.08 x 0.08 mm (without halo)
Distance Focus/last valve	ca. 1068 mm
Height Focus/floor level	ca. 1396.5 mm (1393 mm at the exit of the refocusing chamber)
Free photon beam available	Yes
Fixed end station	No
Higher-harmonics suppression	Different foils are installed in the beamline: Polyimid foil (150 nm thick), Al foil (150 nm thick), and Mg foil (240 nm thick)
Phone number	+49 (30) 8062 -14836 directly at the beamline
Instrument responsible	Prof. Dr. Gregor Schiwietz, schiwietz@helmholtz-berlin.de Dr. Niko Pontius, pontius@helmholtz-berlin.de



The optical layout of the beamline UE112 PGM-1.

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

UE112 PGM-1 - Reference guide for latest publications

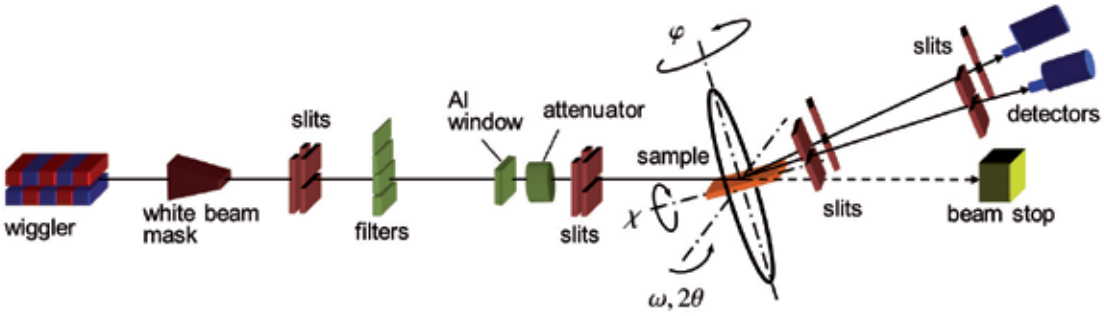
BESSY II

Beamlines Fixed Stations


THORLABS
THORLABS

7T-MPW-EDDI

The beamline is operated in the energy-dispersive mode of diffraction using the direct white photon beam provided by a superconducting 7T multipole wiggler. The wigglers critical energy is 13.5 keV at 1.7 GeV. The figure below shows its energy spectrum recorded directly without any attenuators in the beam by means of a Germanium solid state detector (Canberra).



Instrument application

- Phase analysis (qualitative and quantitative)
- Residual stress analysis
- Texture analysis
- Microstructure analysis (domain sizes and microstrains)
- *In-situ* investigations (*e.g.* under high temperature or external load)
- High spatially resolved measurements (slit widths up to appr. 10 µm possible)
- Simultaneous measurements with two detectors
- Simultaneous radioscopy/tomography and diffraction

References / Latest publications

[1] Genzel, Ch. *et al.*: The Materials Science Synchrotron Beamline EDDI for Energy-Dispersive Diffraction Analysis, Nucl. Instr. and Meth. in Phys. Res. A 578 (2007), 23-33.

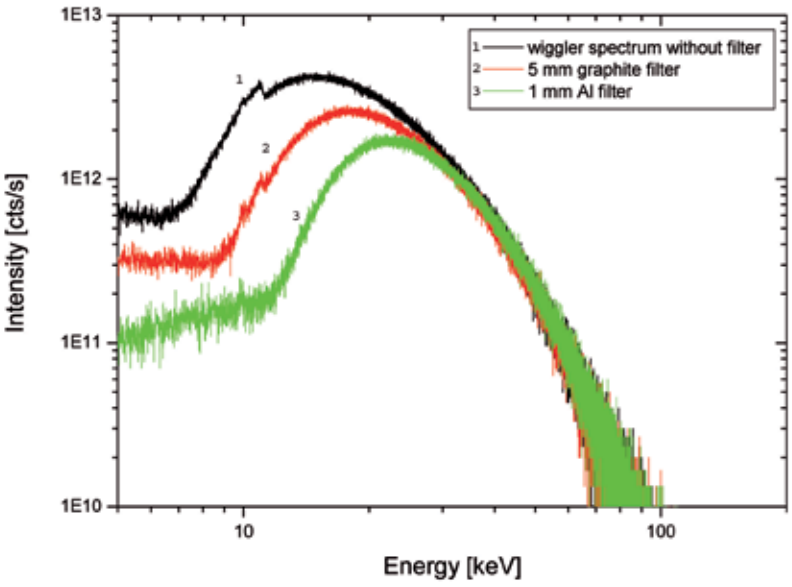
[2] Genzel, Ch. *et al.*: Exploiting the Features of Energy-Dispersive Synchrotron Diffraction for Advanced Residual Stress and Texture Analysis. J. Strain Analysis 46 (2011), 615-625.

[3] Apel, D. *et al.*: Rietveld refinement of energy-dispersive synchrotron measurements. Z. Kristallogr. 226 (2011), 934-943.

[4] García-Moreno, F. *et al.*: White-Beam X-ray Radioscopy and Tomography with Simultaneous Diffraction at the EDDI Beamline, J. Synchrotron Rad. 20 (2013), 809-810.

Instrument data

Location	5.2
Source	7T-MPW
Monochromator	Direct beam (white beam)
Energy range	5 - 150 keV
Energy resolution	Ge solid state detector (Canberra): 160 eV (at 10 keV) and 420 eV (at 100 keV)
Flux	$3 \cdot 10^{12}$ (at 10 keV) and $1 \cdot 10^{10}$ (at 100 keV) (photons/s at 300 mA through a pinhole of 1x1 mm^2)
Polarisation	Horizontal
Divergence horizontal	± 1.2 mrad
Divergence vertical	± 0.5 mrad With a double slit system (30 µm) $\Delta\theta \approx 0.003°$ mrad
Focus size (hor. x vert.)	Focussed beam not possible Beam cross-section: max. 4 x 4 mm^2, usually 0.5-1 mm^2
Distance Focus/last valve	Focussed beam not possible Distance sample/last valve: 6000 mm
Height Focus/floor level	1400 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Manuela Klaus, klaus@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

7T-MPW-EDDI - Reference guide for latest publications

EDDI | Energy Dispersive Diffraction

The experimental station EDDI (Energy Dispersive Diffraction) is a fixed station at the 7T-MPW-EDDI beamline. The beamline provides the direct white photon beam emitted by the 7T multipole wiggler and is operated in the energy-dispersive mode of diffraction. For the experiments two diffractometers with Eularian cradle segments (GE Inspection Technologies) are at the disposal for light and heavy weight samples. For the acquisition of the diffraction patterns as well as the fluorescence signals two Germanium solid state detectors (Canberra) are available.

Instrument application

The flexible EDDI station/beamline is suitable for multi purpose applications, such as:

- Phase analysis (qualitative and quantitative)
- Residual stress analysis
- Texture analysis
- Microstructure analysis (domain sizes and rms microstrains)
- *In-situ* investigations (*e. g.* under high temperature or external load)
- High spatially resolved measurements (slit widths up to appr. 10 µm possible)
- Simultaneous measurements with two detectors

Instrument data

Monochromator	No
Experiment in vacuum	No
Temperature range	Room temperature ... 1100°C (furnace)
Detector	Two Ge solid state detectors (Canberra) resolution: 160 eV (at 10 keV) and 420 eV (at 100 keV)
Manipulators	- 5-axes Eulerian cradle (for samples up to 1 - 2 kg) - 4-axes Eularian cradle (for samples up to 50 kg) - Hexapod (PI GmbH) - Tensile-compressive loading device (Walter+Bai) up to ±20 kN furnace (Anton-Paar DHS 1100) between 25°C and 1100°C - Two detector setup possible - Other sample environments and user sample environments possible
Energy range	White beam (range between 5 keV and 150 keV)
Instrument responsible	Dr. Manuela Klaus, klaus@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

References / Latest publications

[1] Denks, I. A., Genzel, Ch.: Enhancement of energy-dispersive residual stress analysis by consideration of detector electronic effects, Nucl. Instrum. Methods in Phys. Research B 262 (2007), 87-94.

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EDDI - Reference guide for latest publications

7T-MPW-SAXS/WAXS

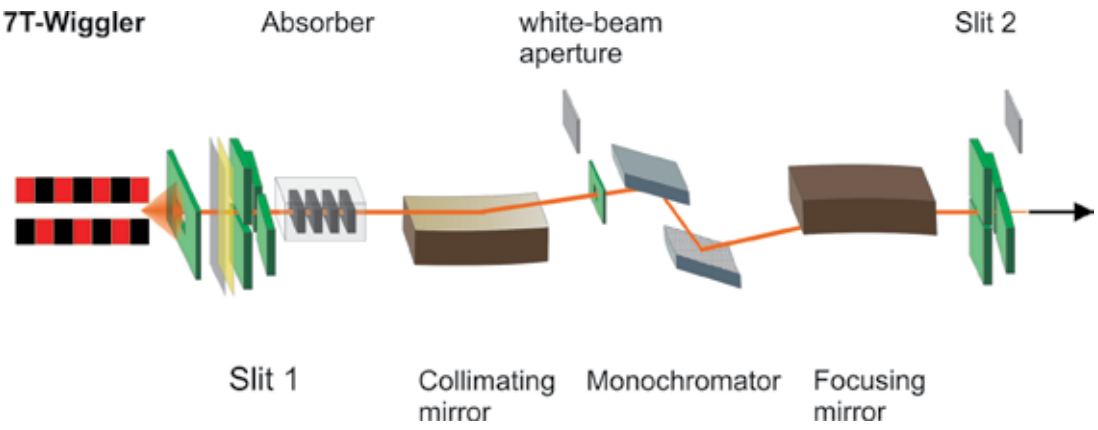
The beamline provides a monochromatic beam of X-rays in the range from about 3.5 keV to 30 keV. The X-ray source is a 7 Tesla multipole superconducting wiggler with a critical energy of 13.4 keV at current operating conditions of BESSY II (1.7 GeV). The beamline optics consist of a Si(111) double crystal monochromator and a pair of retractable collimating and focusing mirrors. The optics is bendable to provide flexible horizontal and vertical focusing.
The available user beamtime is right now offered for small angle X-ray scattering experiments (SAXS), favoring ASAXS.

Instrument application

- ASAXS, SAXS, GISAXS, WAXS

Instrument data

Location	5.2
Source	7T-Multipole Wiggler
Monochromator	Si(111) DCM
Energy range	3.5 - 30 keV
Energy resolution	$\Delta E/E \sim 2 \cdot 10^{-4}$
Flux	10^{13} - 10^{11} photons/s (flux at 10 keV)
Polarization	Horizontal
Divergence horizontal	5.1 mrad
Divergence vertical	0.56 mrad
Focus size (hor. x vert.)	1.2 x 0.4 mm
Distance Focus/last valve	Flexible
Height Focus/floor level	1373 mm
Free photon beam available	Only under special conditions
Fixed end station	No
Instrument responsible	Dr. Armin Hoell, hoell@helmholtz-berlin.de PD Dr. Günter Goerigk, guenter.goerigk@helmholtz-berlin.de



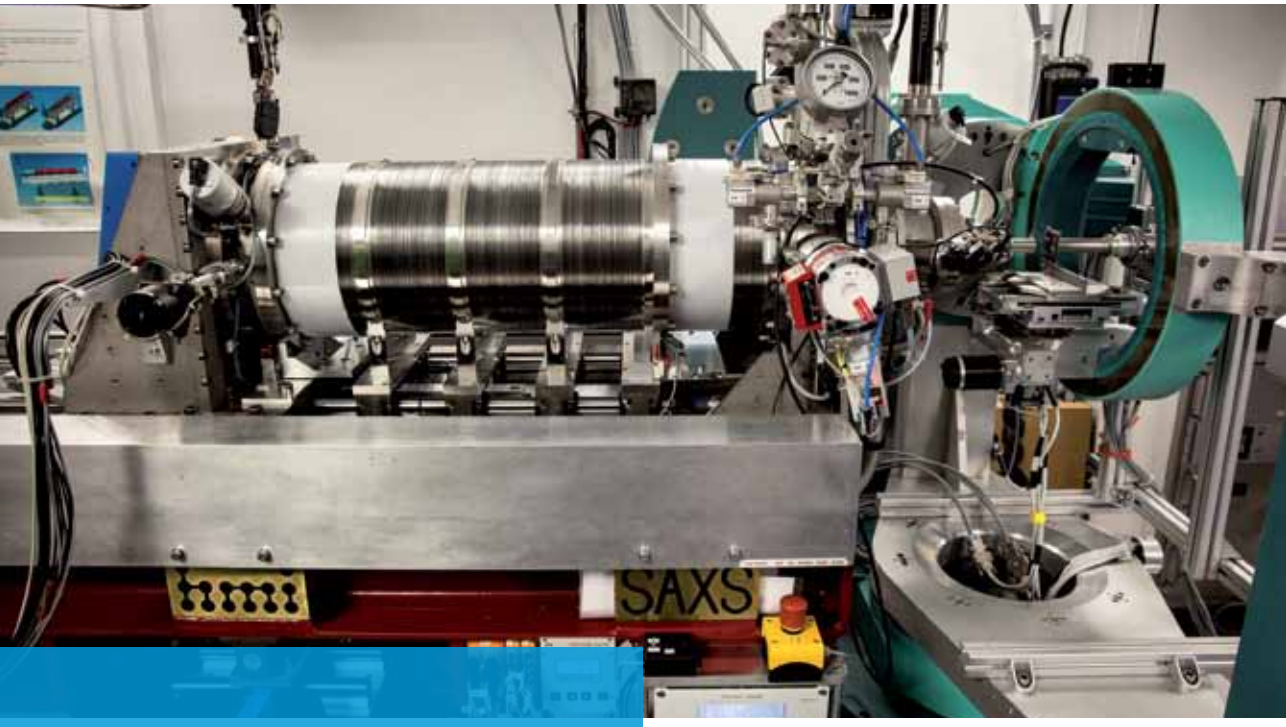
EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Dudzik, E. *et al.*: The new HMI beamline MAGS: an instrument for hard X-ray diffraction at BESSY, J. Synchrotron Rad. 13 (2006), 421-425.

7T-MPW-SAXS/WAXS - Reference guide for latest publications



SAXS/ASAXS | Small Angle X-ray Scattering

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

The SAXS instrument is designed for Anomalous Small Angle X-ray Scattering (ASAXS) and also for Grazing Incidence SAXS (GISAXS). A combination of both techniques is possible. ASAXS provides exceptional possibilities by combining the element-specific structural size analysis with a quantitative analysis of volume fractions and chemical concentrations in nano-scaled phases. The method is sensitive on a length scale from just above the atomic size up to several 100 nanometres. It can be used in chemistry, physics, biology, materials science and catalyst research like critical phenomena, kinetics of phase transitions, self-assembling, transport phenomena and catalytic activity. The ASAXS instrument is an end-station at the monochromatic branch of the 7T-Multipole Wiggler source.

The main features of the SAXS instrument construction (patent: DE 10 2006 029 449) are an optical bench that can be tilted and a continuously varying sample-detector distance. Both movements are independent and automated. The main construction detail is an edge welded bellow system between the sample position and the SAXS area detector. The entire instrument can be moved easily in and out of beam position on an own air cushion system. Monitor counters and diodes for absorption measurements allowing precise transmission measurements and calibrations of the scattering signal.

Instrument data

Monochromator	Fixed-exit double crystal monochromator Si(111), sagitally focusing second crystal
Experiment in vacuum	Yes
Detector	Multiple scattering detectors available
Manipulators	See sample environments
Source type	7 T cryogenic wiggler
Energy range for SAXS	3.8 keV to 27.5 keV
Energy resolution	$\Delta E / E \sim 2 \cdot 10^{-4}$
Scattering Detectors	1. Multi-wire proportional counter gas detector, 20 · 20 cm^2 2. Mar CCD165
Sample – detector distance	0.78 - 3.75 m (continuously variable)
Beam size at sample; typically	300 x 300 μm^2
Flux	$3 \cdot 10^{12}$ at 300 mA, 10 keV photons/s
q-range	0.05 – 3.6 (at 5 keV) nm^{-1} 0.10 – 7.2 (at 10 keV) nm^{-1} 0.25 – 18.4 (at 25 keV) nm^{-1}
Dimensions	1.8 - 125 (at 5 keV) nm 0.9 - 62 (at 10 keV) nm 0.4 - 25 (at 25 keV) nm
Sample environments	1. Sample changer under vacuum environment (standard setup) 2. Sample changer under air condition 3. Sample furnace on a sample changer: T= 300 K - 970 K; usable under vacuum or under air conditions 4. High temperature furnace: T= 550 K - 1450 K; usable under vacuum and some gas atmospheres 5. Cryo-furnace: T= 50 K - 320 K; vacuum conditions 6. Sample changer for capillaries with a thermostat 260 K to 370 K 7. GISAXS setup under air condition 8. Free places for user-owned sample environments
Special environments of users	1. Ultrasonic trap 2. Different electrochemical cells for catalysis 3. Microfluidic setup 4. GISAXS in combination with a furnace and an ellipsometer
Instrument responsible	Dr. Armin Hoell, hoell@helmholtz-berlin.de PD Dr. Günter Goerigk, guenter.goerigk@helmholtz-berlin.de

Instrument application

- Nanostructured metal alloys, glasses, semiconductor alloys: photovoltaic
- Porous materials and catalysts: dry house reforming of greenhouse gases
- Soft matter systems, polyelectrolytes: Conformation of macromolecular structures
- Technical and bio-membranes: fuel cell applications and bio-reactors for the synthesis of functional nanoparticles

References / Latest publications

[1] Haas, S. *et al.*: Direct Accessing the Nanostructure of Carbon Supported Ru–Se Based Catalysts by ASAXS, J. Phys. Chem. C 114 (2010), 22375-22384.

[2] Haas, S. *et al.*: Analysis of nanostructure and nanochemistry by ASAXS: Accessing phase composition of oxyfluoride glass ceramics doped with Er^{3+}/Yb^{3+}, Phys. Rev. B 81 (2010), 184207.

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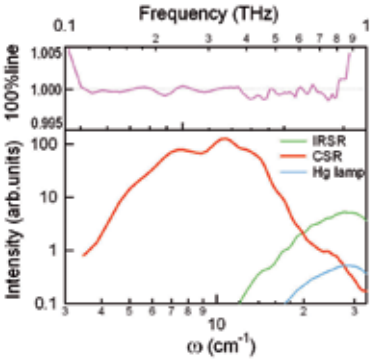
SAXS/ASAXS - Reference guide for latest publications

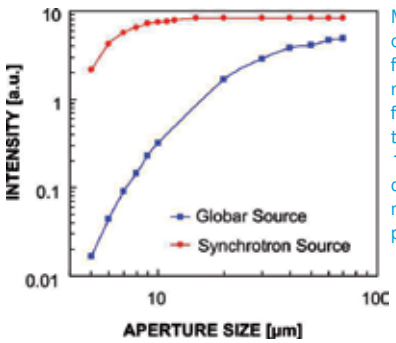
IRIS THz/IR

At synchrotron light sources of third generation like BESSY II the emitted radiation in the infrared wavelength region is some orders of magnitude brighter than standard thermal broadband sources (*e.g.*, globar). In addition, infrared synchrotron radiation is an absolute source being polarized and pulsed in the picosecond timescale. As a particular speciality, BESSY II provides a new technique (low-alpha) to generate high power, stabile and low-noise Coherent Terahertz (THz) Radiation.

The IRIS Beamline at BESSY was inaugurated in December 2001. The large acceptance, multipurpose beamline delivers broadband infrared radiation from the THz to the NIR and is used by a multi-disciplinary community.



Running BESSY II in the low-alpha mode yields coherent synchrotron radiation (CSR) at the IRIS beamline with fluxes orders of magnitudes higher than obtained with incoherent infrared synchrotron radiation (IRSR) or with internal spectrometer sources (Hg lamp.)



More than one order of magnitude more flux in the mid infrared range can be fed through apertures smaller than 10 x 10 µm^2 making diffraction-limited microspectroscopy possible.

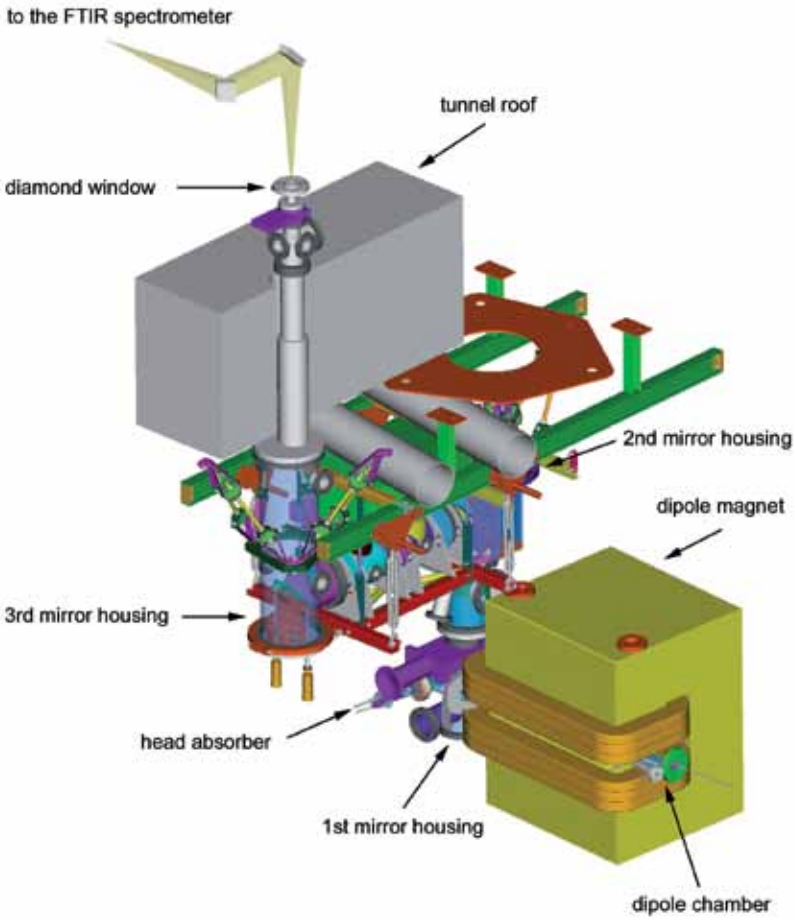
Instrument data

Location	3.1
Source	D11
Monochromator	Fourier Transform Spectrometers
Energy range	0.0006-1 eV, 2-10000 1/cm, 0.1-300 THz
Energy resolution	0.125 1/cm
Polarisation	Linearilly horizontal/vertical
Divergence horizontal	60 mrad
Divergence vertical	40 mrad
Focus size (hor. x vert.)	Diffraction limited
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Ulrich Schade, ulrich.schade@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

IRIS THz - Reference guide for latest publications



References / Latest publications

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IR-Spectrometer and Microscopy

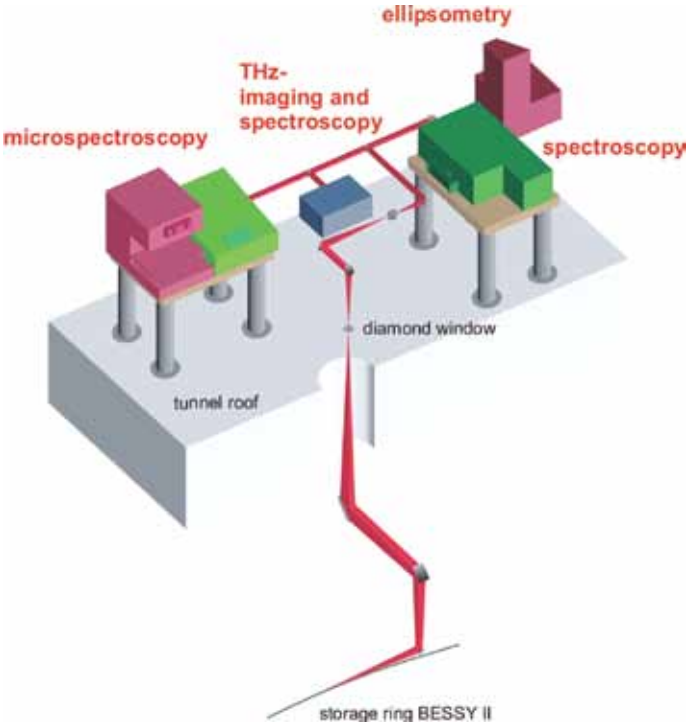
With the unique characteristics of the infrared synchrotron radiation source from the mid to the far infrared and THz spectral range, it is possible to perform new and exciting experiments in material and life sciences at the multipurpose infrared beamline IRIS.
Several fixed end-stations are ready for the users; among them are Fourier-transform infrared (FT-IR) spectrometers (Bruker 66/v, Thermo Nicolet Nexus™ 470 and 4700, in-house built Martin-Puplett spectrometer), an infrared microscope (Thermo Nicolet Continuμm) and a mid-infrared mapping ellipsometer (developed at ISAS Berlin). In addition, a free beam port is applicable for own bread-boarding experiments.

Instrument application

The end-stations at IRIS can be used for manifold spectroscopic investigations, *e.g.*, of biological systems (cells, tissues, fibres), for diffraction-limited microscopy of same and for the investigations on the structural and functional interactions of proteins. In addition, vibrational, structural and electronic properties of liquids, solids, surfaces and thin layers can be studied. This allows addressing scientific problems in the fields from cultural heritages to novel materials under a broad variety of environmental conditions. The in-house developed far-infrared microscope attachment enables the users to investigate phase transitions of matter upon high pressure. The high brilliance in the THz spectral range is used to study the optical conductivity at low temperatures of small-sized and unique single crystalline samples of novel materials, *e.g.*, high-T_c superconductors.

Instrument data

Monochromator	Fourier Transform Spectrometers
Experiment in vacuum	Yes
Temperature range	1.6K - 500 K
Detector	Bolometer, DTGS, MCT, InSb, Si
Manipulators	Cryostat
Instrument responsible	Dr. Ulrich Schade ulrich.schade@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

IR Spectrometer - Reference guide for latest publications

References / Latest publications

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HIKE | High Kinetic Energy Photoelectron Spectroscopy

The HIKE end-station has been set-up in late 2005 and begun user operation in 2006. The system is designed for hard X-ray high kinetic energy photoelectron spectroscopy (HAXPES or HIKE) experiments using a photon excitation energy range from 2 keV to 12 keV with an optimized available photoelectron kinetic energy range from 150 eV to 10000 eV.

While soft X-ray photoelectron spectroscopy *e.g.* ESCA is one of the most important spectroscopic tools of today due to its surface sensitivity, HAXPES goes beyond the surface and probes the true bulk electronic properties of materials. The technique insensitivity to surface effects and contaminants allows the study of samples without particular surface treatments such as prototype systems for applications such as magnetic memories, solar cells, batteries etc. .

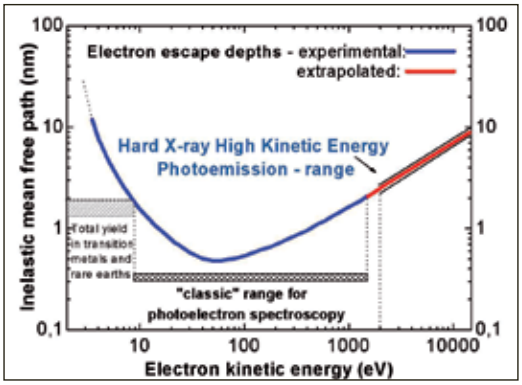
The HIKE end-station is installed at the KMC-1 beamline. Typical experiments running on the HIKE end station are investigations of bulk samples, multilayers and heterostructures where core levels and valence band are recorded, buried interfaces are accessed and spatially resolved chemical information by X-ray standing waves is recorded. In addition to HAXPES experiments the station also provides parallel access to the sample drain current (TEY) and the signal from a fluorescence detector (FY) thus enabling absorption experiments: XANES and EXAFS.

Instrument application

- Extended depth profiling yielding stoichiometry and chemistry information
- Buried interface chemistry investigations *e.g.* diffusion, order disorder transitions
- Standing waves enhanced HAXPES

Instrument data

Monochromator	Double crystal @ KMC-1
Experiment in vacuum	Yes
Temperature range	Tested: 112 K - 1023 K
Detector	VG Scienta R4000 electron analyzer, Bruker XFlash® 4010 fluorescence detector
Manipulators	VG Scienta He cryostat with 5 degrees of freedom - 4 motorized
Manipulator motorization	Axis X, Y, Z, Polar - Labview controlled
Sample transfer	Omicron type
Sputter gun	Yes, Available gas: Argon
Charge compensation flood gun	Yes - with electron energies up to 300 eV
X-ray Focusing	Glass Capillary X-ray Optics: parabolic X-ray mono-capillary (IfG GmbH) Beam properties @ experiment: Focus: 100 microns x 50 microns; Flux density gain: x15; HIKE overall signal gain: x5.
Instrument responsible	Dr. Mihaela Gorgoi, mihaela.gorgoi@helmholtz-berlin.de



References / Latest publications

[1] Holmström, E. *et al.*: A Sample Preserving Deep Interface Characterisation Technique, Phys. Rev. Lett. 97 (2006), 266106.

[2] Sing, M. *et al.*: Profiling the Interface Electron Gas of $LaAlO_3/SrTiO_3$ Heterostructures with Hard X-ray Photoelectron Spectroscopy, Phys. Rev. Lett. 102 (2009), 176805.

[3] Philippe, B. *et al.*: Improved performances of nano-silicon electrodes using the salt LiFSI: a photoelectron spectroscopy study, J. Am. Chem. Soc. 135 (2013), 9829.

[4] Gorgoi, M. *et al.*: High Kinetic Energy Photoelectron Spectroscopy Facility at BESSY: Progress and First Results, Nucl. Instr. Meth. Phys. Res. A 601 (2009), 48-53.

HIKE - Reference guide for latest publications

KMC-2

The beamline provides an experimental set-up for EXAFS, XANES, and X-ray fluorescence measurements at-air in the energy range of 4 keV – 15 keV. Beam intensity is stabilized by MOSTAB electronics with an accuracy of 0.3 %. At end station KMC-2 XANES, the detector system consists of three ionization chambers, a Si-PIN photodiode for fluorescence measurements, a scintillation counter and an energy-dispersive detector (Röntec X-Flash). An add-on microprobe capillary system with the spatial resolution of >3.6 µm is available for micro-EXAFS, micro-fluorescence and micro-diffraction experiments.

At end station DIFFRACTION, for X-Ray diffractometry and reflectometry the experimental hutch is equipped with a 6-axis HUBER goniometer and a 2-dimensional cross-wire detector with a spatial resolution of 150 µm. In addition detectors listed are available. A high-resolution X-ray CCD camera with a pixel size of 6.7 µm can be used for experimental alignment.

Instrument application

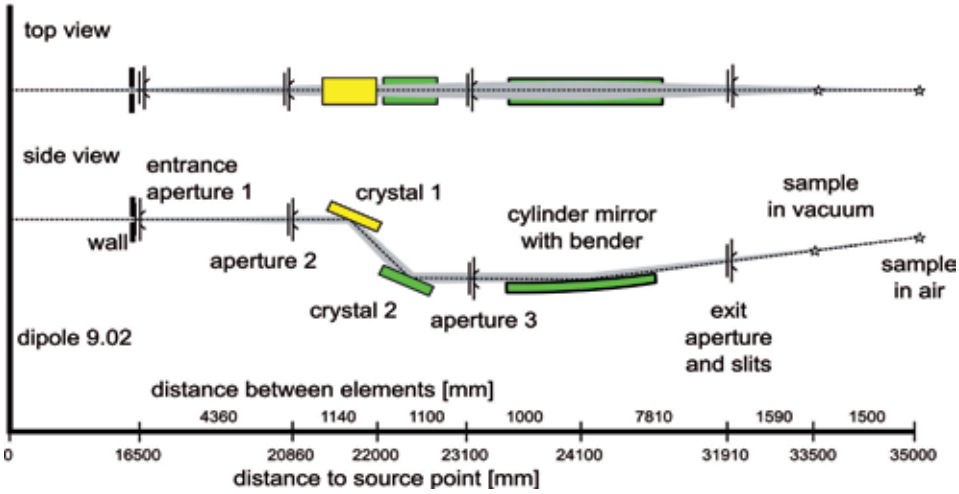
- EXAFS measurements
- XANES measurements
- Fluorescence measurements
- Micro-XANES
- Micro-fluorescence
- Fluorescence mapping
- Grazing incidence diffraction (GID)
- Reciprocal space mapping of single crystal Bragg reflections
- Diffuse scattering
- Powder diffraction
- Anomalous diffraction
- Reflectometry

Materials

- Liquids, molecular solutions, liquid crystals
- Single- and poly-crystalline materials
- Amorphous and highly disordered solids
- Molecules and macromolecules containing metallic atoms or partially substituted with heavy atoms

Instrument data

Location	11.1
Source	D9.2
Monochromator	KMC
Energy range	5 - 14 keV
Energy resolution	4000
Flux	10^7 - 10^{10}
Polarisation	Horizontal
Divergence horizontal	2.5 mrad
Divergence vertical	0.5 mrad
Focus size (hor. x vert.)	250 µm x 600 µm (4.8 µm x 4.8 µm with capillary optics)
Distance Focus/last valve	2500 mm
Height Focus/floor level	1465-1490 (depending on lateral position) mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Daniel Többens, daniel.toebbens@helmholtz-berlin.de



References

[1] Erko, A. *et al.*: The Crystal Monochromator Based on graded SiGe Crystals, Nuclear Instruments and Methods in Physics Research A467-468 (2001), 358-361.

[2] Erko, A. *et al.*: KMC-2: the new X-ray beamline at BESSY II, AIP Conference Proceedings 521 (2000), 415-418.

KMC-2 - Reference guide for latest publications

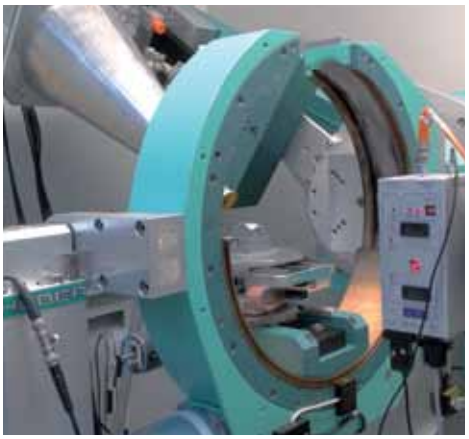
KMC-2 Diffraction

The station Diffraction is a flexible multi-purpose diffractometer. The very variable configuration of the instrument covers most scattering requirements.

A Huber six circle diffractometer in psi geometry is the central part of the experiment. Two detectors are available: A scintillation point detector (Cyberstar) with motorized detector apertures allows high resolution experiments. A MikroGap area detector (Bruker Våntec 2000) provides reciprocal space coverage with high counting rates and low background. The sample is mounted on a motorized stage allowing movement in all three directions as well as rotation. Diffraction is located at the KMC-2 beamline, which provides X-ray radiation with very stable energies in the range between 4 and 14 keV.
This instrument setup allows a wide range of diffraction experiments, including grazing incidence diffraction (GID), reciprocal space mapping of single crystal Bragg reflections, diffuse scattering, powder diffraction, anomalous diffraction, and measurements of reflectivity.
A high temperature vacuum chamber (up to 1000 °C) is available to perform *in-situ* experiments. The chamber is equipped with a Be-Dome and provides vacuum down to 10^{-6} mbar also at high temperatures. A low temperature cryostat and a cryofurnace are also available, and user-provided sample environments can be easily adapted. The operation system spec has external trigger to act as master system for accordingly equipped analytical devices.

Exemplary instrument applications

- Lattice misfits in superalloys by reciprocal space mapping of selected Bragg reflections
- *In-situ* determination of lattice spacing and phase composition of nanoporous gold films during loading with lithium ions
- Surface acoustic wave propagation in piezoelectric crystals
- *In-situ* gas adsorption into metal-organic frameworks (MOFs)
- Point defect concentration in photovoltaic sulfides from Rietveld refinement of anomalous scattering data
- Phase separation in p-doped thin polymer films from grazing incidence diffraction (GID)



Instrument data

Monochromator	Ge-graded Si(111) (KMC-2)
Experiment in vacuum	No
Temperature range	6 - 1273 K
Diffraction angle 2θ	0 - 140°
Point detector	Cyberstar Scintillator, motorized & manual apertures
Area detector	Bruker Våntec 2000 MikroGap, 14 cm x 14 cm active area, 2048 x 2048 pixels, 250 µm spatial resolution
Goniometer	Huber, six circle psi-geometry, open Eulerian cradle
Sample stage	Huber XY-stage (5102.18) + Z-stage
Instrument responsible	Dr. Daniel Többens, daniel.toebbens@helmholtz-berlin.de

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KMC-2 Diffraction - Reference guide for latest publications

Selected publications

[1] Bon, V. *et al.*: *In-situ* observation of gating phenomena in the flexible porous coordination polymer $Zn_2(BPnDC)_2(bpy)$ (SNU-9) in a combined diffraction and gas adsorption experiment. Inorganic Chemistry, 53 (2014), 1513-1520.

[2] Roshchupkin, D. *et al.*: X-ray diffraction study of surface acoustic waves and pseudo-surface acoustic waves propagation in $La_3Ga_{5.5}Ta_{0.5}O_{14}$ crystal, Journal of Applied Physics 113 (2013), 144909.

[3] Jenichen, B. *et al.*: Residual disorder and diffusion in thin Heusler alloy films. Physical Review B 86 (2012), 075319.

KMC-2 XANES

The KMC-2 XANES is a dedicated endstation to investigate the short-range environment around selected atomic species in condensed matter by X-ray Absorption Spectroscopy. This end-station provides possibility for EXAFS, XANES and X-ray fluorescence measurements at-air. The detector system consists of three ionization chambers, Si-PIN photodiode, energy-dispersive detector (Röntec X-Flash) and scintillation counter. An add-on microprobe capillary system with the spatial resolution of > 1 µm is available for micro XAFS and micro-fluorescence experiments. A high-resolution X-ray CCD camera with a pixel size of 6.7 µm can be used for experimental alignment.

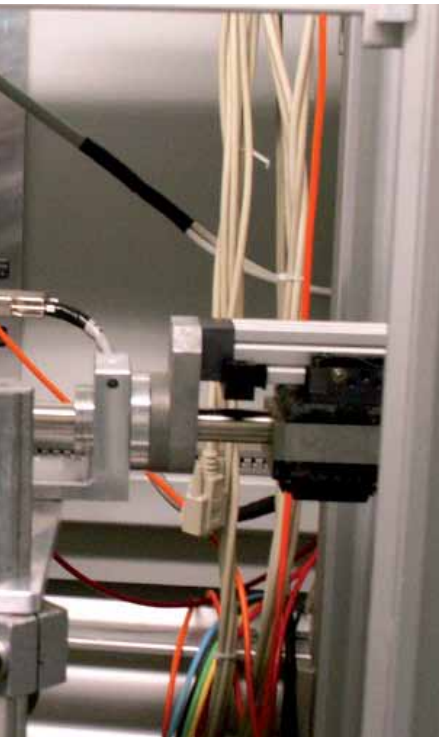
The experimental setup allows for a parallel monitoring of the transmitted through the sample X-ray beam intensity as well as for fluorescence yield measurements. This end-station is permanently attached to the KMC-2 beamline providing medium photon flux between 4000 eV and 15000 eV and linear photon polarization, necessary to exploit the potential of X-ray absorption spectroscopy.

Instrument application

X-ray Absorption Spectroscopy (XAS) is a powerful structural technique to investigate the short-range environment around selected atomic species in condensed matter. While scanning the X-ray energy impinging onto the sample, a core level photoelectron is generated. This is scattered by the surroundings matter producing interference effects visible in the absorption cross-section and usually referred to as X-ray absorption fine structure (XAFS). The process itself is general and therefore fundamental to study structural properties in materials like:

- Liquids, molecular solutions, liquid crystals
- Single- and poly-crystalline materials
- Amorphous and highly disordered solids
- Molecules and macromolecules containing metallic atoms or partially substituted with heavy atoms

The energy range 4.0 keV < E < 15 keV is suitable for K-edge studies of elements in the range 21 < Z < 36 and L-edge studies of elements in the range 49 < Z < 83. The sample thicknesses for experiments are in the µm range for transmission experiments. Studies on thin film and dilute systems are possible in fluorescence mode.



EXPERIMENTAL HALL BESSY II

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KMC-2 XANES - Reference guide for latest publications

Selected publications

[1] Preda, I. *et al.*: X-ray absorption study of the local structure at the NiO/oxide interfaces. J. Synchr. Rad. 20 (2013), 635-640.

[2] Liu, Y. *et al.*: Local structure and site substitution in $Al_{86}Ni_6Co_2Y_{4.5}La_{1.5}$ bulk amorphous alloy. Materials Letters, 70 (2012), 171-173.

[3] Katsikini, M. *et al.*: Comparison of Fe and Si doping of GaN: An EXAFS and Raman study. Materials Science and Engineering B 176 (2011), 723-726.

Instrument data

Monochromator	KMC-2
Experiment in vacuum	No
Temperature range	293 K
Detector	Röntec X-Flash, 3 ionization chambers, Si-PIN photodiodes
Manipulators	Huber goniometer
Beam intensity stabilization	MOSTAB electronics (accuracy 0.3%)
Microfocusing	> 1 µm
Micro-EXAFS, micro-fluorescen	Yes
Maximum sample size	Unlimited
Control system	PC-based BESSY monochromator control system EMP/2
Data-acquisition computer	Personal computer, measurement bus-extension, OS/2-operating system
Data-acquisition software	Windows-NT, RADICON RDPW software
Instrument responsible	Dr. Stefan Zander, stefan.zander@helmholtz-berlin.de

KMC-3 XPP

The XPP/KMC-3 is a hard X-ray beamline dedicated to time-resolved X-ray diffraction and absorption spectroscopy experiments (EXAFS, XANES). It is equipped with an X-ray mirror assembly and a double monochromator, which can be removed from the X-ray beam path to allow for experiments with a monochromatic or a white X-ray beam. The energy range extends from 2 keV to 14 keV. In addition, the beamline comprises an ultrafast laser as a pump source for time-resolved experiments. In the near furture, a four-circle diffractometer setup in a vacuum chamber will allow for sample cooling down to 30 K.

Instrument application

Ultrafast X-ray Diffraction in solid state and soft matter systems:

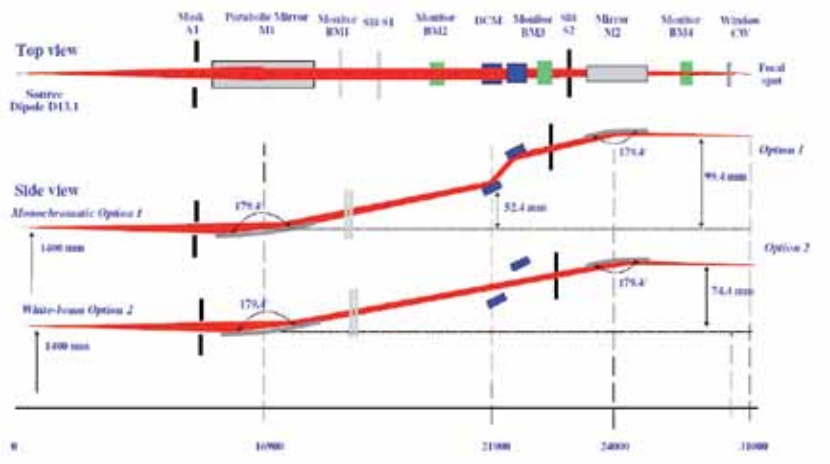
- Heat diffusion in nanoscale systems
- Coherent lattice dynamics
- Electronic and magnetic coupling to the crystal structure in multiferroic systems
- Phasetransitions and phase change materials
- Diagnostics for hard X-rays

Cryo-EXAFS / XANES / Fluorescence measurements:

- Liquids, molecular solutions and liquid crystals
- Single- and polychristalline materials
- Amorphous and highly disordered solids
- Molecules and macromolecules

Instrument data

Location	15.1
Source	D21
Monochromator	KMC-3
Energy range	2 – 14 keV
Energy resolution	1/1000 - 1/5000
Flux	10^{11} photons/s
Polarisation	Horizontal
Focus size (hor. x vert.)	150 x 400 µm^2
Height Focus/floor level	1480 mm
Fixed end station	No
Instrument responsible	Dr. Peter Gaal, peter.gaal@helmholtz-berlin.de Dr. Maria Brzhezinskaya, maria.brzhezinskaya@helmholtz-berlin.de



References / Latest publications

[1] Gaal, P. *et al.*: Ultrafast Switching of hard X-rays, J. Synchrotron Rad. 21 (2014), 2, 380-385.

[2] Gaal, P. *et al.*: Time-domain sampling of X-ray pulses using an ultrafast sample response, Appl. Phys. Lett. 101 (2012), 24, 243106.

[3] Shayduk, R. *et al.*: Direct time-domain sampling of subterahertz coherent acoustic phonon spectra in SrTiO3 using ultrafast X-ray diffraction, Phys. Rev. B 87 (2013), 18, 184301.

[4] Navirian, H. *et al.*: Synchrotron-based ultrafast X-ray diffraction at high repetition rates, Rev. Sci. Instrum. 83 (2012), 6, 063303.

[5] Shayduk, R. *et al.*: Nanoscale heat transport studied by high-resolution time-resolved X-ray diffraction, New J. Phys. 13 (2011), 9, 093032.

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BEAMLINES BESSY II

KMC-3 XPP - Reference guide for latest publications

XPP | X-ray Pump Probe

The XPP station is dedicated to ultrafast X-ray diffraction (UXRD) experiments at high repetition rates. It comprises a four-axes goniometer which is mounted in a vacuum vessel and a cryostat for sample cooling. Optical pump light and the X-ray probe pulses enter the vacuum chamber on quasi collinear beam paths. The goniometer axes allow scanning of a large reciprocal space volume while preserving the illuminated pump area on the sample surface. Hence, several in-plane and out-of-plane diffraction peaks can be measured under comparable optical pump conditions.

The setup is specifically optimized for experiments at high laser repetition rates where fast heat removal from the excited samples is required. The setup provides two cooling options: 1) The sample holder is connected to a cryostat via flexible copper wires. While allowing full

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mechanical flexibility the sample can be cooled down to temperatures of 30 K.
2) The excited sample surface can be directly cooled with a cooled nitrogen jet. The temperature range of the coolant extends from room temperature to 90 K. This configuration can either be used for efficient heat removal from the excited sample or for real cooling to cryogenic temperatures. Samples are excited by ultrafast optical pulses emitted from an ytterbium-doped fiber laser. Laser parameters are listed below. Alternative excitation concepts are currently developed, *e.g.*, sample excitation with ultrashort current or voltage pulses.
The XPP-station is currently in an upgrade / commissioning phase. If you wish to apply for beamtime, please contact the Beamline scientist in advance to discuss the feasibility of your experiment.

Instrument data

The laser source is a multi-stage ytterbium-doped oscillator - amplifier system (Impulse, Clark-MXR). It is synchronized to the RF-signal of the storage ring with accuracy better than 5 ps. The main laser parameters are:

Pulse energy	10 µJ
Pulse duration	250 fs
Center wavelength	1030 nm
Repetition rate	200 kHz - 1.25 MHz (adjustable)
Temperature range and sample cooling options	• 30 - 300 K: fixed cryostat in vacuum vessel • 90 - 450 K: nitrogen jet
Operation	Wavelength conversion via sum and difference frequency mixing and parametric amplification
Instrument responsible	Dr. Peter Gaal, peter.gaal@helmholtz-berlin.de

Instrument application

- Heat diffusion in nanoscale systems
- Coherent lattice dynamics
- Electronic and magnetic coupling to the crystal structure in multiferroic systems
- Phasetransitions and phase change materials
- Diagnostics for hard X-rays

XPP - Reference guide for latest publications

References / Latest publications

[1] Gaal, P. *et al.*: Ultrafast switching of hard X-rays, J. Synchrotron Rad., 21 (2014), 2, 380-385.

[2] Gaal, P. *et al.*: Time-domain sampling of an X-ray pulse using an ultrafast sample response, APL 101 (2012), 243106.

[3] Shayduk, R. *et al.*: Direct time domain sampling of sub-THz coherent acoustic phonon spectra in SrTiO3 using ultrafast X-ray diffraction, Phys. Rev. B, 87 (2013), 18, 184301.

[4] Shayduk, R. *et al.*: Nanoscale heat transport studied by high-resolution time-resolved X-ray diffraction, NJP 13 (2011), 093032.

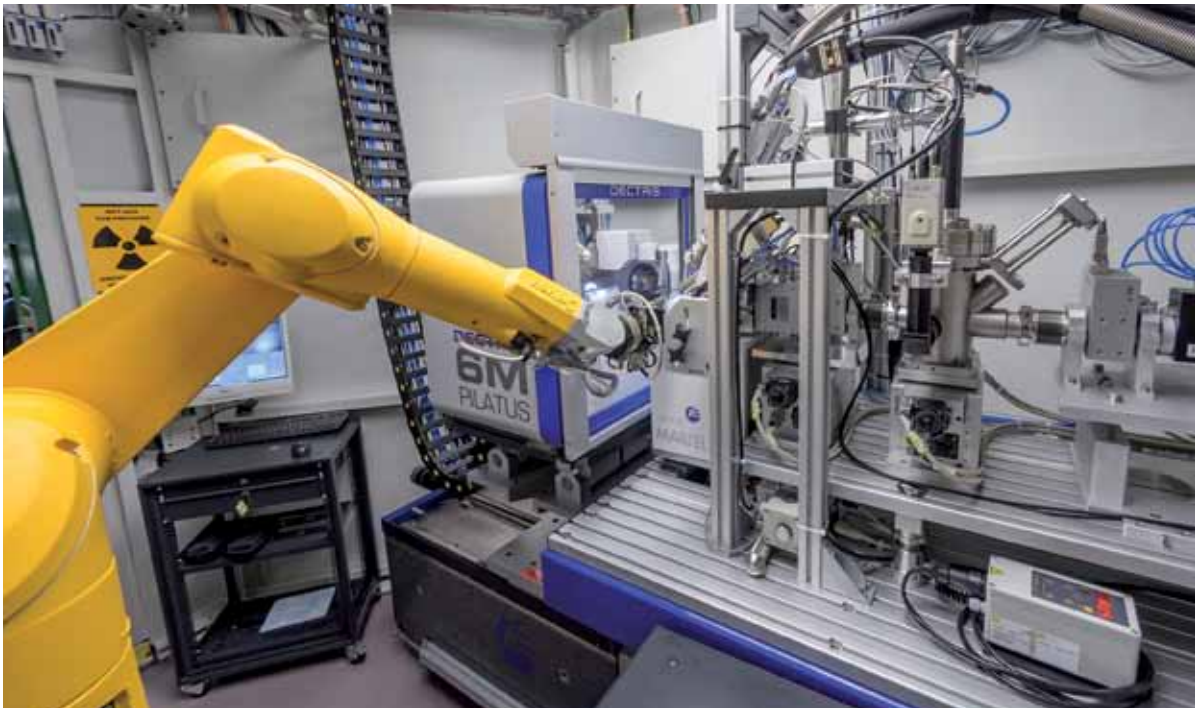
MX BL 14.1 and **end-station**

BL 14.1 is a tuneable energy beamline dedicated to macromolecular crystallography. This beamline is highly automated and can support X-ray diffraction experiments of small crystals up to 15 micrometers. Samples may be mounted using a CATS sample changer robot (IRELEC, France). Rapid data collection experiments are possible with the PILATUS 6M pixel-detector (DECTRIS, Switzerland).

BL 14.2, BL 14.3 and BL 14.1 from left to right within the optics hutch

Instrument application

- *De novo* structure determination using MAD, SAD
- High throughput screening for drug discovery
- Qualitative element analysis by X-ray fluorescence
- Long wavelength phasing
- UV radiation damage phasing
- Noble gas based phasing and solvent channel mapping



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MX BL 14.1 - Reference guide for latest publications

Instrument data

Location	15.2
Source	7T-WLS-2
Monochromator	KMC-1
Energy range	5 - 15.5 keV
Energy resolution	2 eV
Flux	$1.4 \cdot 10^{11}$ (Photons/s/100mA)
Polarization	Horizontal
Divergence horizontal	0.5 mrad
Divergence vertical	0.5 mrad
Focus size (hor. x vert.)	170x90 μm^2 110x90 μm^2 80x70 μm^2 60x50 μm^2 40x30 μm^2
Free photon beam available	Yes
Fixed end station	Yes
Monochromator	Si111-DCM with sagital bender
Experiment in vacuum	No
Temperature range	90 - 293 K
Detector	• X-fluoresence detector: Roentec X-Flash • Pixel-detector: Pilatus 6M
Manipulators	CATS sample changer
Goniometer	Microdiffractometer MD2 with Minikappa goniometer MK3
Instrument responsible	Dr. Uwe Müller, umue@helmholtz-berlin.de Dr. Manfred Weiss, manfred.weiss@helmholtz-berlin.de

References / Latest publications

[1] Smietanski, M. *et al.*, Structural analysis of human 2'-O-ribose methyltransferases involved in mRNA cap structure formation, Nature Communications 5 (2014), 3004.

[2] Lüdtke, S. *et al.*: Sub-angstrom-resolution crystallography reveals physical distortions that enhance reactivity of a covalent enzymatic intermediate, Nat. Chem. 5 (2013), 762-767.

[3] Mueller, U. *et al.*: Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin, J. Synch. Rad., 19 (2012), 442-449.

MX BL 14.2 and **end-station**

BL14.2 is a tuneable energy beamline dedicated to macromolecular crystallography. This beamline is a work horse instrument for many X-ray diffraction experimental applications for macromolecular and small molecule structure determinations. Both high-resolution and long-wavelength experiments are supported by this beamline. Rapid data collections are possible with the MX225 ccd detector (Rayonix, USA).

BL14.2 experimental station

Instrument application

- *De novo* structure determination using MAD, SAD
- Qualitative Element analysis by X-ray fluorescence
- Long wavelength phasing
- Atomic resolution data collection for macromolecules and small molecules
- Noble gas based phasing and solvent channel mapping

MX BL 14.2 - Reference guide for latest publications

Instrument data

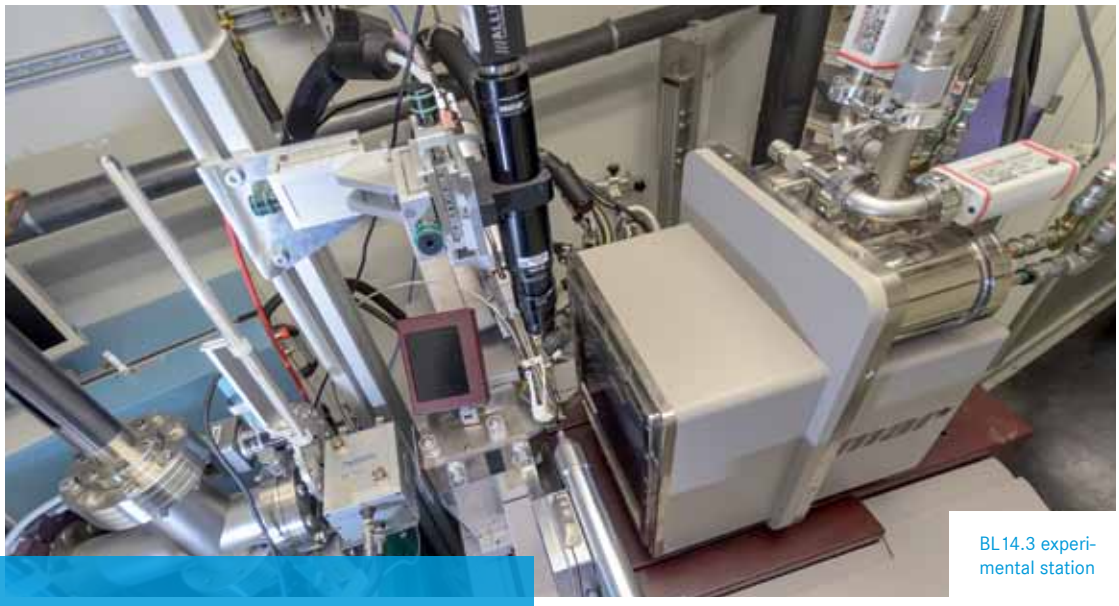
Location	15.2
Source	7T-WLS-2
Monochromator	KMC-2
Energy range	5 - 15.5 keV
Energy resolution	2 eV
Flux	$1.9 \cdot 10^{11}$ (Phot/s/100mA/0.05% BW)
Polarization	Horizontal
Divergence horizontal	0.5 mrad
Divergence vertical	0.5 mrad
Focus size (hor. x vert.)	180x70 μm^2
Free photon beam available	Yes
Fixed end station	Yes
Monochromator	Si111 DCM with sagital bender
Experiment in vacuum	No
Temperature range	90 - 293 K
Detector	• X-fluoresence detector: Amptek • Pixel-detector: MX-225
Manipulators	No
Goniometer	marresearch dtb
Instrument responsible	Dr. Uwe Müller, umue@helmholtz-berlin.de Dr. Manfred Weiss, manfred.weiss@helmholtz-berlin.de

References / Latest publications

[1] Liebscher, S. *et al.*: N-Terminal Protein Modification by Substrate-Activated Reverse Proteolysis, Angewandte Chemie Int Ed Engl, 53 (2014), 3024-3028.

[2] Frielingsdorf, S. *et al.*: Reversible [4Fe-3S] cluster morphing in an O2-tolerant [NiFe] hydrogenase, Nature Chem. Biol. 10 (2014), 378-85.

[3] Mueller, U. *et al.*: Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin, J. Synch. Rad., 19 (2012), 442-449.



BL 14.3 experimental station

MX BL 14.3 and **end-station**

BL 14.3 is a fixed energy beamline operated at 13.8 keV and is dedicated to macromolecular crystallography. This beamline is a work horse instrument for many X-ray diffraction experimental applications for macromolecular and small molecule structure determinations. Fast data collections are possible with the MX225 ccd detector (Rayonix, USA). Additionally, this beamline offers the controlled dehydration of crystalline samples using the HC 1c dehydration system (ARINAX, France).

BL 14.3 beamline exit system with photon shutter and slit system

Instrument application

- *De novo* structure determination using SAD
- Controlled crystal dehydration with HC1c
- Crystal screening
- Atomic resolution data collection for macromolecules and small molecules
- Noble gas based phasing and solvent channel mapping

MX BL 14.3 - Reference guide for latest publications

Instrument data

Location	15.2
Source	7T-WLS-2
Monochromator	KMC-3
Energy range	13.87 keV
Energy resolution	5 eV
Flux	$0.4 \cdot 10^{11}$ (Phot/s/100mA/0.05% BW)
Polarization	Horizontal
Divergence horizontal	2.5 mrad
Divergence vertical	2.5 mrad
Focus size (hor. x vert.)	180x110 μm^2
Free photon beam available	No
Fixed end station	No
Monochromator	Si111 single crystal monochromator with direct water cooling
Experiment in vacuum	No
Temperature range	90 - 293 K
Detector	• X-fluoresence detector: Amptek CR100 • Pixel-detector: MX-225
Manipulators	No
Goniometer	marresearch dtb
Instrument responsible	Dr. Uwe Müller, umue@helmholtz-berlin.de Dr. Manfred Weiss, manfred.weiss@helmholtz-berlin.de

References / Latest publications

[1] Zebisch, M. *et al.*: Crystallographic Snapshots along the Reaction Pathway of Nucleoside Triphosphate Diphosphohydrolases, Structure 21 (2013),1460-1475.

[2] Hoeppner, A. *et al.*: Structure of the corrinoid: coenzyme M methyltransferase MtaA from Methanosarcina mazei, Acta Crystallogr D 68 (2012),1549-1557.

[3] Mueller, U. *et al.*: Facilities for Macromolecular Crystallography at the Helmholtz-Zentrum Berlin, J. Synch. Rad., 19 (2012), 442-449.

mySpot Beamline

mySpot beamline is used to provide stable beam especially tuned for the mySpot experiment. Depending on the experiment requirements, different optical devices are used. The schematic view shows two different configurations, one tuned for low divergence, and one for narrow energy band width, as required for the scattering and spectroscopy experiments respectively. Since the goal of the experiment is to provide several methods at the same time, beamline properties can be tuned to provide the optimal beam for a given combination of experiments. Total intensity, divergence, energy resolution, high harmonics suppression, and stability in scans can be tuned to match the requirements. For details, please visit the experiment page.

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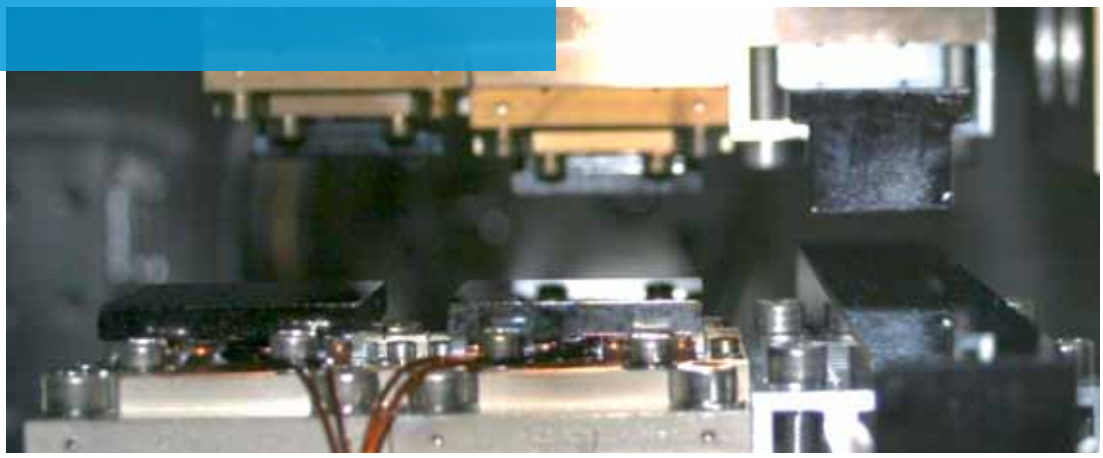
3 monochromators of the mySpot Beamline, left to right: Si111, Si311, B4C/Mo Multilayer



Instrument application

The main purpose of the mySpot beamline is to provide photons for the mySpot experiment. All the beamline parameters can be tuned from the experiment.

Low divergence application: The second mirror is not used. The beam is focused hirisontally and vertically directly to the sample position. Beam size is 400x400 μm^2. This creates additional energy band broadening, and can not be combined with XANES experiment.

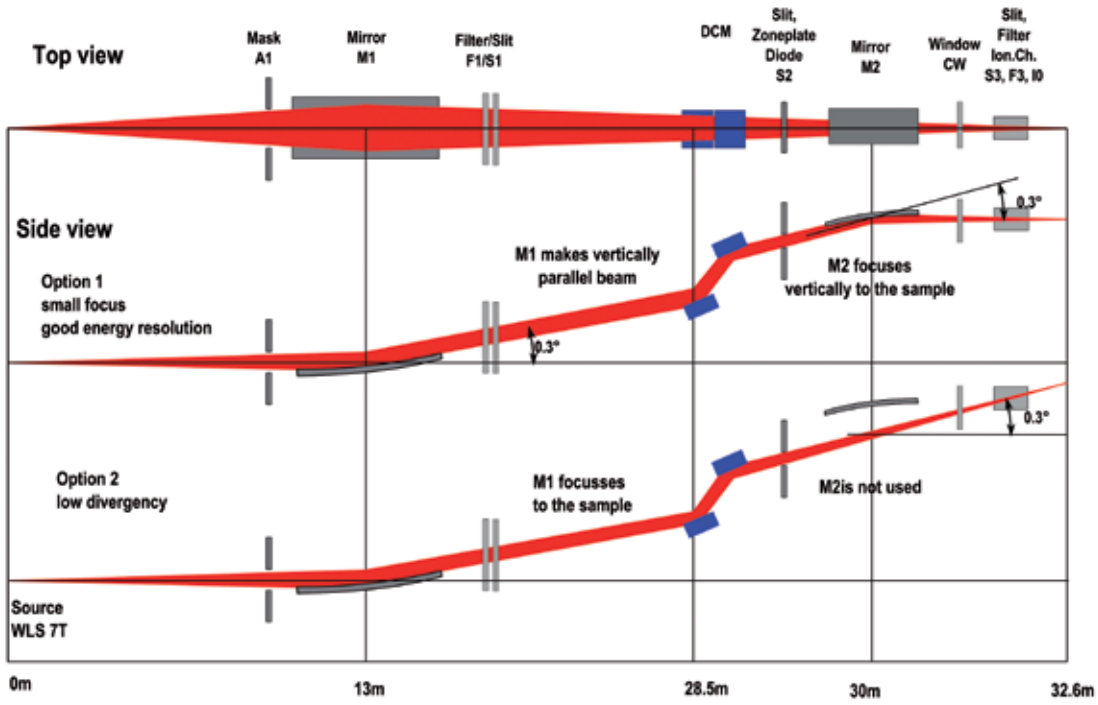
Narrow energy bandwidth: First mirror is used to parallelize the beam, so there is no additional broadening in the monochromator. Second mirror is focusing the beam at the sample position. Beam size at the sample position is 400x50 μm^2. Additionally, a Si (311) crystal pair is used for low energy bandwidth. Unfortunately, this influences the total intensity.

High flux option: A multilayer monochromator is used when there is no requirement on the energy bandwidth, like in diffuse scattering and fluorescence mapping.
The second mirror has three different coatings, which can be used to suppress the higher harmonics to ensure the beam purity for different energy ranges.

To provide the extreme stability during the energy scans, the monochromator is operated in a servo loop using the feedback from the beam intensity monitor at the end of the beamline.
For microfocussing experiments with the beam size down to 1 μm^2, the beam is additionally refocused very close to the sample using single bounce or capillary optics. Small distance between the sample and focusing optics provides for the extreme vibration and position stability during the scans, ao that micro-EXAFS and micro-XANES experiment are possible. See the experiment page for more details.

Instrument data

Location	3.2
Source	7T-WLS-1
Monochromator	Si(111) and Si(111) crystal monochromator/ Mo-B4C Multilayer
Energy range	4 – 30 keV (not all energies are available for all experiments)
Energy resolution	ΔE/E depending on monochomator: from 1/500 to 1/10000
Flux	10^{12} – 10^{13}, depending on monochromator and optics
Polarization	Horizontal
Divergence horizontal	1 mrad
Divergence vertical	1 mrad
Focus size (hor. x vert.)	400x400, 400x50, further focusing in experimental hutch
Distance Focus/last valve	Variable mm
Height Focus/floor level	1500 mm
Free photon beam available	No, beamline dedicated to mySpot experiment
Fixed end station	Yes, mySpot
Instrument responsible	Dr. Ivo Zizak, zizak@helmholtz-berlin.de Dr. Maria Brzhezinskaya, maria.brzhezinskaya@helmholtz-berlin.de



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mySpot - Reference guide for latest publications

Synchrotron Facility BESSY II

mySpot | MPG

µ-XANES, -EXAFS, -XRF, -SAXS, -WAXS, -Raman

mySpot is a versatile microfocussing station for scanning methods with resolution down to 1.5 µm, providing a combination of methods which can be performed simultaneously at the same sample position. It is especially designed (but not limited to) for the study of hierarchically structured biological samples. Structural information from different scales (XRD - crystalline, SAXS - nanometer, Video-microscope - micrometer, sample translation - milimeter) can be combined with chemical information (XRF-mapping, EXAFS, XANES) and molecular information (Raman) providing unique insight into the mutual dependencies of different parameters.

The beamline provides focal spot of about 500x50 µm, which can be refocused at the sample using capillary optics. Capillary optics is used for two main reasons: 1) the focal spot does not depend on the energy which makes EXAFS and XANES measurements very simple, and 2) the optics is positioned very close to the sample which improves the stability of the focus at the sample.

This makes the focal spot of 1.5 µm in 2D scans possible, as well as very parallel beam for scattering experiments down to 10µm, or volume element of 20 µm diameter for 3D XRF mapping.

Instrument data

Monochromator	Selective Si311, Si111, Multilayer
Experiment in vacuum	No
Temperature range	180 - 320 K
Detector	Several ionisation chambers and calibrated PIN Diodes, 7-channel Si(Li) energy dispersive detector (210 mm^2 area), Si-Drift energy dispersive det. (100 mm^2 area), Mar X-ray CCD area detector for scattering, Renishaw Raman spektrometer, Ocean Optics Raman Spectrometer, CCD (visible light) built in the online microscope
Manipulators	Several goniometers and translation stages, to be used depending on the sample size
Energy range	6 - 30 keV as excitation for XRF, for spectroscopy 5-25 keV
Energy band width Si111	4000 E / ΔE
Energy band width ML	500 E / ΔE
Energy band width Si311	8000 E / ΔE
Raman options	Parallel with X-ray beam, normal to the sample surface
Raman wavelength	532 and 785 nm
Instrument responsible	Dr. Ivo Zizak, zizak@helmholtz-berlin.de

Instrument application

The mySpot beamline is specialized for mapping experiments using different methods. Depending on the required method the focus varies between 1.5 and 100 µm. Most methods can be combined. However, the user should take into account that the beam requirements vary for different methods. Example: For XRF mapping with 1.5 µm focus the beam is strongly focused to the sample, providing enough intensity to perform even EXAFS at selected positions. If small angle scattering from the same position is required, this strong focusing is not possible, rendering simultaneous microEXAFS and SAXS with 1.5 µm focal spot very complicated.

Following methods are available and can be combined with restrictions:

1) micro-XRF mapping. Detectors available: 7 channel Si(Li) detector with 210 mm^2 surface or 80 mm^2 Silicon drift detector. The smaller detector is used for combined scattering/XRF measurements. Resolution depends on the used optics and can be selected between 1.5 and 20µm. Primary beam energy range is 6 keV-25 keV.

2) 3D XRF-Mapping. 7 channel detector is used, although only one channel is assigned to the volume mapping. This allows for the acquisition of the fluorescence signal from different directions and estimation of the inelastic scattering. For this method we use polycapillaries with focal distance of about 3 mm and focal spot of about 15 µm.

3) X-ray scattering. SAXS and WAXS signal can be acquired using a CCD camera positioned downstram from the sample. Maximal scattering angle is 45°, resolution in SAXS regime is 100 nm^{-1}. This provides structural information at the crystalline and nanometer scale.

4) micro-EXAFS and XANES. Capillary optics allows the acquisition of the energy-dependent absorption spectra on selected position at the sample.

5) Visible/NIR Raman scattering. It is possible to acquire Raman spectra in combination with X-ray measurements. For this two different Raman systems are available. In-line Renishaw Raman spectrometer (in cooperation with MPIKG Golm) allows for very precise Raman spectra to be acquired, using laser excitation parallel to the X-ray beam. For the combination with XRF measurements, a smaller, faster (down to 0.1 s per spectrum) system can be mounted where the laser excitation is illuminating the sample at the 45° with respect to the X-ray beam. Both systems provide wavelengths 532 and 785 nm.

6) Optical microscope is available for alignment purposes, but the microscopy images can be saved at every measurement coordinate, so that the correlation between the measured data and the microscopy is rather simple.

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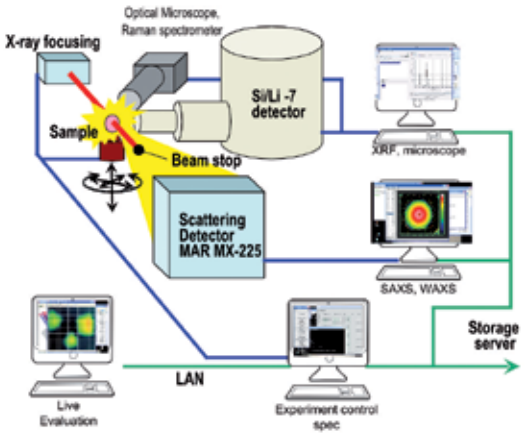
Sample environments:

Different scanning environments for different sample sizes (from several micrometer to 150 mm) are available at the beamline. Rotational units are available for both scattering and fluorescence methods.
There is no vacuum environment available at the beamline, but it is possible to mount sample environments or reactors at the available 1-circle goniometer in the experimental hutch. Different experiments were successfully mounted at the station, including *in-situ* stretching devices, plasma chambers, laser-levitation sample holders...

Sample cooling for very small samples (~1 mm) is available through cryo stram down to -150°C. For larger samples (~1 cm) a Linkam cryo-scanning chamber is available, providing temperatures between Liquid Nitrogen and 200°C. Only clean, non-gasing samples are accepted for heating experiments.
Temperature and humidity in experimental hutch are controlled to provide non-destructive atmosphere for sensible samples. For information about complicated measurements and combination of methods please contact the beamline scientist.



Data acquisition schematic for the mapping experiment. All the detectors are simultaneously evaluated and the data can be imediately evaluated for the better planning of the next steps.

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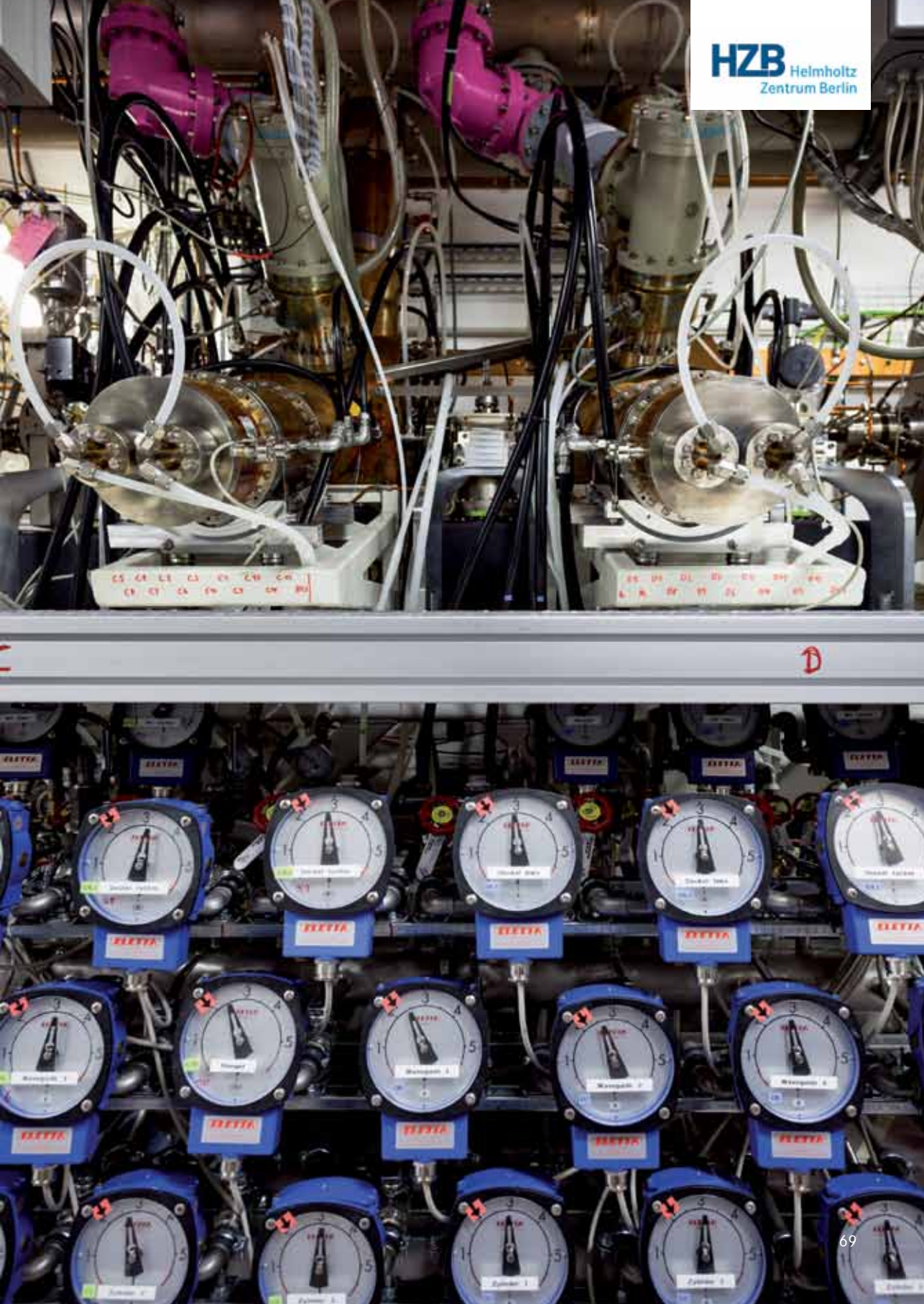
mySpot - Reference guide
for latest publications



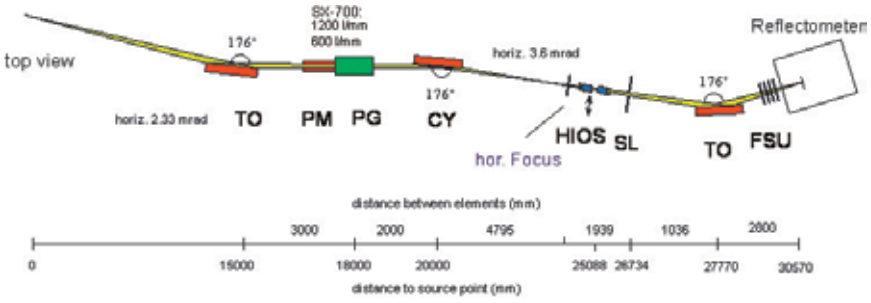
HZB Helmholtz Zentrum Berlin

Optics Beamline PM-1

The Optics Beamline PM-1 at the BESSY II dipole 1.1 is dedicated to at-wavelength characterization and calibration of the in-house produced diffraction gratings and nano-optical devices as well as to the input control of mirrors and multilayer systems. It is coupled to a versatile 4-circle UHV-Reflectometer as a permanent end station which is located in a moderate clean-room hutch and which allows to carry out Reflectometry experiments on a very high precision level. The Plane Grating Monochromator (PGM) beamline is operated in collimated light. The SX700 monochromator is equipped by newly produced blazed gratings (600 and 1200 l/mm). Over the operating range from 10 to 2000 eV this bending magnet beamline has very high spectral purity achieved by a four-mirror arrangement of different coatings which can be inserted into the beam path at different angles and by absorber filters for high order suppression. Stray light and scattered radiation is removed efficiently by *in-situ* exchangeable apertures and slits.

Instrument application

- At Wavelength metrology (quality control) of XUV-optics: Multilayers, mirrors, gratings, zoneplates, crystals, thin films
- Reflectivity, efficiency, transmission, diffraction
- Scattering (specular - non specular)
- Non-destructive investigation and characterisation of optical surfaces
- In depth analysis of internal material structure including buried layers and interfaces
- Optical constants derived from accurate reflectivity measurements



Instrument data

Location	Section DIP 1.1
Source	Dipole
Monochromator (gratings)	SX700 (600 l/mm, 1200 l/mm)
Energy range	10 eV - 2000 eV
Energy resolution	E/ΔE= 1000 - 10000
Flux	10^{10} - 10^{11} photons/s/100 mA
Polarization	Horizontal-linear, elliptical
Divergence horizontal	3.5 mrad
Divergence vertical	0.5 mrad
Focus size (hor. x vert.)	0.3 x 0.2 mm^2
Distance Focus/last valve	1290 mm
Height Focus/floor level	1430 mm
Free photon beam available	No
Fixed end station	4-circle UHV-Reflectometer
Absorption filters	Mg, Al, Be, B, C_6H_8, Ti, Cr, Fe, Cu
HiOS mirrors coatings	Si, AlF_3, C
Instrument responsible	Dr. Andrey Sokolov, andrey.sokolov@helmholtz-berlin.de Dr. Franz Schäfers, franz.schaefers@helmholtz-berlin.de

References / Latest publications

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EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

Optics Beamline PM-1 - Reference guide for latest publications

Reflectometer | Reflectometry Station

The 4-circule UHV-Reflectometer is a versatile precision instrument for at-wavelength metrology and calibration of XUV optical elements: gratings, novel nano-optical devices, input control of mirrors and multilayer systems. The main feature of this Reflectometer is the possibility to incorporate large samples (up to 4 kg and 360 mm in length) into the UHV-chamber. The samples are adjustable within six degrees of freedom by a novel UHV- compact tripod system. The reflectivity can be measured between -180° and +180° incidence angle for both s- and p-polarisation geometry by azimuthal rotation of the sample around the beam direction. A variety of in-situ exchangeable detectors with different angular resolution and dynamic range are available in the setup. The Reflectometer is located in a moderate clean-room hutch at the experimental floor of BESSY II and is permanently attached to the Optics Beamline PM1 at Dipole 1.1, of which the optical design was matched to reflectometry requirements: high spectral and stray light purity, large working energy range, low divergence of incident beam at moderate energy resolution.

Instrument data

Monochromator	Optics Beamline – PM1
Experiment in vacuum	10^{-9} mbar
Max. sample size	360 x 60 x 60 mm^3
Max. sample size for LoadLock	50 x 50 x 10 mm^3
Maximum sample weight	4 kg
Sample surface scan	15 x 15 mm
Incidence angle scan range	$-180° \leq \theta \leq 180°$
Azimuthal angle scan range	$0° \leq \beta \leq 360°$
Detector scan range (in plane)	$-180° \leq 2\theta \leq 180°$
(off-plane)	$-4° \leq \Theta_D \leq 4°$
Min. step size for all motors	0.001°
Sample – Detector Distance	310 mm
Detector	GaAsP-photodiode with Keithley electrometer 617 (6514)
Detectors size	4 x 4 mm^2, slits or pinholes: 0.14 – 4 mm
Instrument responsible	Dr. Andrey Sokolov, andrey.sokolov@helmholtz-berlin.de Dr. Franz Schäfers, franz.schaefers@helmholtz-berlin.de

Instrument application

- At Wavelength metrology (quality control)
- Multilayers, mirrors, gratings, zoneplates, crystals, thin films
- Reflectivity, efficiency, transmission, diffraction
- Scattering (specular - non specular)
- Non-destructive characterisation of optical surfaces
- Internal material structure including buried layers
- Interface quality
- Optical constants

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Reflectometer - Reference guide for latest publications

PM4

This soft X-ray bending magnet beamline is equipped with a Plane Grating Monochromator operated in collimated light (collimated PGM). Since summer 2014 the beamline is equipped with a new permanent Low Dose Photoemission (LowDosePES) end station. The MHz mechanical chopper will be installed at the position of the intermediate horizontal focus, enabling permanent access to 1.25 MHz pulsed X-rays during regular hybrid mode operation.

Instrument application

Organic semiconductors have unique functionality for printable and flexible electronics, photovoltaic and highly efficient light emitting diodes. But high conversion efficiency and performance requires a tailored bulk and interface electronic structure. Direct measurement is very challenging, due to the very high sensitivity to radiation damage.

With a three orders of magnitude higher transmission the Low Dose Photoemission station will be a unique facility for angular and time resolved photoemission experiments on radiation damage sensitive samples. The new station will be based on the modern angular resolving time-of-flight electron spectrometers and versatile X-ray pulse picking schemes.

Instrument data

Location	10.1
Source	D81
Monochromator	PGM
Energy range	20 eV - 2000 eV
Energy resolution	6000 at 400 eV
Flux	10^9 - 10^{10} photons/s
Polarisation	Horizontal
Divergence horizontal	1.5 mrad
Divergence vertical	1.0 mrad
Focus size (hor. x vert.)	0.3 x 0.09 mm^2
Distance Focus/last valve	1050 mm
Height Focus/floor level	1415 mm
Free photon beam available	No
Instrument responsible	Dr. Ruslan Ovsyannikov, ovsyannikov@helmholtz-berlin.de

References / Latest publications

[1] Nau, S. *et al.*: Highly efficient color-stable deep-blue multilayer PLEDs: preventing PEDOT:PSS-induced interface degradation. Adv. Mater. 25 (2013), 4420-4.

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EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

PM4 - Reference guide for latest publications

LowDose PES | Low-Dose Photoelectron Spectroscopy

The new LowDose PES end station is installed at BESSY II PM-4 beamline. The station is equipped with a SES100 hemispherical analyser as well as a novel angle-resolved time-of-flight ArTOF spectrometer. The extreme high transmission of the ArTOF spectrometer facilitates investigations of samples at a much reduced photon flux, and allows a considerable reduction of the total measurement time. In addition to the decrease of the beam exposure, the ArTOF makes it possible to cover a broad angular range in parallel. A pulsed source with a repetition rate of up to a few MHz required by the ArTOF spectrometer will be accomplished by a MHz mechanical chopper which will be installed at the position of the intermediate horizontal focus of the beamline, enabling a permanent access to 1.25 MHz pulsed X-rays during regular hybrid mode operation.

Instrument data

Monochromator	PGM, energy range: 18 to 1800 eV
Experiment in vacuum	Yes
Temperature range	10-400 K
Detector	Scienta ArTOF 10k electron energy analyser , SES100 electron energy analyzer
Manipulators	VG x,y,z,θ stage with Janis cryostat
Sample	Maximum size 10 mm x 10 mm, thickness up to 3mm
Top preparation chamber	Clean sample preparation, up to 3 replaceable evaporators can be installed, LEED, mass spectrometer
First prep. chamber (clean)	Non-organic preparation chamber, sample heating to 900 K, two gas inlets, sputter gun, quartz microbalance and a port for replaceable evaporator
Second prep. chamber (organics)	Organic preparation chamber, sample heating to 900 K, two replaceable evaporators, quartz microbalance and mass spectrometer.
Instrument responsible	Dr. Ruslan Ovsyannikov, ovsyannikov@helmholtz-berlin.de

Instrument application

Using ArTOF analyser 1000 times faster acquisition times and equally reduced dose rates can be achieved, which gives a new look at crucial electronic properties such as band structure of hybrid and photoactive organic materials. Using such low dose PES investigations, the acquisition can be performed in a few hours, making such experiments feasible for a much wider class of systems. The fast acquisition rate as well as the full cone detection of the ArTOF analyser allow to track changes in the sample electronic structure as a function of parameters such as temperature or gas exposure.

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Applications of the instrument include:

- Electronic structure of organic semiconductors, molecular magnets and etc
- ARPES on extremely radiation sensetive organic single crystals
- Orbital tomography
- Structural and chemical information via X-ray Photoelectron Diffraction

LowDose PES - Reference guide for latest publications

U41 TXM

This beamline is dedicated to X-ray microscopy applications and hosts the X-ray microscope.

The optical design of the HZB full-field TXM at the BESSY II undulator beamline U41-FSGM allows high spectral resolution of E/ΔE = 10000, 25 nm (half-pitch) spatial resolution and field of views in the range of 10-15 µm. A focusing spherical grating monochromator provides the high energy resolution. The X-ray condenser (ellipsoidal shaped capillary) illuminates the object while the high resolving zone plate objective forms the enlarged image onto the CCD.

Details about the TXM itself can be found in the list of stations under XM - X-ray microscopy.

Instrument application

- X-ray nano-tomography
  - of cells
  - of porous materials
- NEXAFS-TXM (nano-spectroscopy) of nanoscale materials
- Electromigration and stress migration in semiconductors
- Dichroism in materials

Instrument data

Location	Segment 12 - near pillar 13.2
Source	U41
Monochromator	FSGM a
Energy range	250 - 1500 eV
Energy resolution	Up to 10000
Flux	$2 \cdot 10^{12}$ photons/sec @100 mA and 10 µm exit slit; $3 \cdot 10^{8}$ photons/(sec·µm^2) @100 mA and 10 µm exit slit on the sample
Polarization	Horizontal
Divergence horizontal	Photon energy dependent: 0.2 - 0.1 mrad
Divergence vertical	Photon energy dependent: 0.66 - 0.25 mrad
Focus size (hor. x vert.)	220 µm in exit slit
Distance Focus/last valve	In exit slit mm
Height Focus/floor level	1370 mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Peter Guttmann, peter.guttmann@helmholtz-berlin.de Dr. Stephan Werner, stephan.werner@helmholtz-berlin.de

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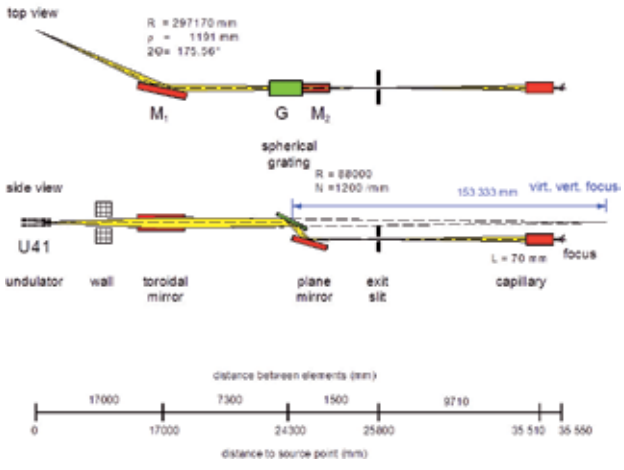
U41 TXM - Reference guide for latest publications



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XM – X-ray Microscopy

In the nano-ages new tools for the analysis of complex structures are essential. The HZB-microscopy group develops novel methods for X-ray imaging to make use out of the unique interactions of X-rays with matter. For this, X-ray optics for the 10 nm scale characterization of the nanostructure, chemical nature, and composition of materials with high energy resolution are engineered and fabricated. We have developed a novel full-field transmission X-ray microscope (TXM) for the soft X-ray range that uses partially-coherent object illumination instead of the quasi-coherent illumination used in earlier setups.

This TXM had demonstrated its high potential for life sciences by nano-tomography of cryogenic samples. High resolution images of cryogenic thick biological specimens with 3-D resolution around 30 nm (half-pitch) have been achieved. Additionally, due to the high energy resolution spatially-resolved NEXAFS studies (NEXAFS-TXM) for material sciences are possible.

An incorporated fluorescence light microscope was developed. This permits to record fluorescence, bright field and DIC images of cryogenic samples (cells) inside the TXM. Thus, two complementary imaging modalities are available and allow correlative studies.

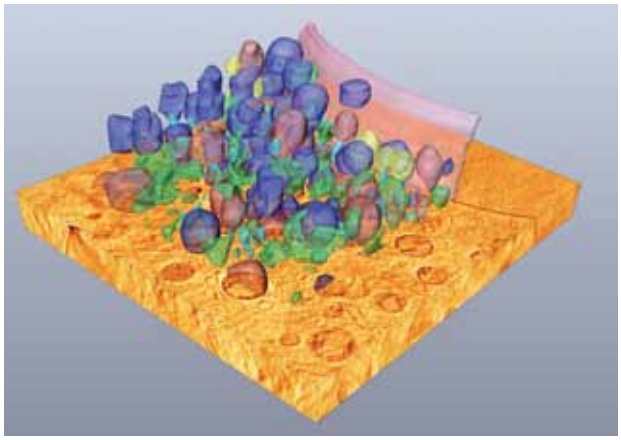
The new optical design of the TXM at the BESSY II undulator beamline U41-FSGM allows high spectral resolution of $E/\Delta E$ = 10000, 25 nm (half-pitch) spatial resolution and field of views in the range of 10 - 15 µm. Using the third order of diffraction of a zone plate objective with 20 nm outermost zone width fabricated at the HZB (using our advanced electron beam lithography system EBPG5000plusES from Vistec), 11 nm lines and spaces of a multilayer test structure were clearly resolved.

Instrument data

Monochromator	U41-FSGM
Experiment in vacuum	Yes
Temperature range	100 K to room temperature
Detector	Thinned, backside illuminated CCD, 1340 pixel x 1300 pixel (Roper Scientific)
Manipulators	Goniometer - CompuStage (FEI)
Tomography capability	Tilt range -80° to +80°
Instrument responsible	Dr. Peter Guttmann, peter.guttmann@helmholtz-berlin.de Dr. Stephan Werner, stephan.werner@helmholtz-berlin.de

Instrument application

- Cryo nano-tomography of cells
- Nano-tomography of porous materials
- Nano-spectroscopy: NEXAFS-TXM of nanoscale materials
- Electromigration and stress migration in semiconductors
- Dichroism in nanoscale materials



Three-dimensional reconstruction of a mouse adenocarcinoma cells at ~36 nm (Rayleigh) resolution allows by volumetric rendering of the cell cytoplasm to visualize many subcellular organelles including mitochondria (M), lyosomes (L), endoplasmic reticulum (ER), vesicles (V), the plasma membrane (PM), the nuclear membrane (NM). [Ref.: 3]

References / Latest publications

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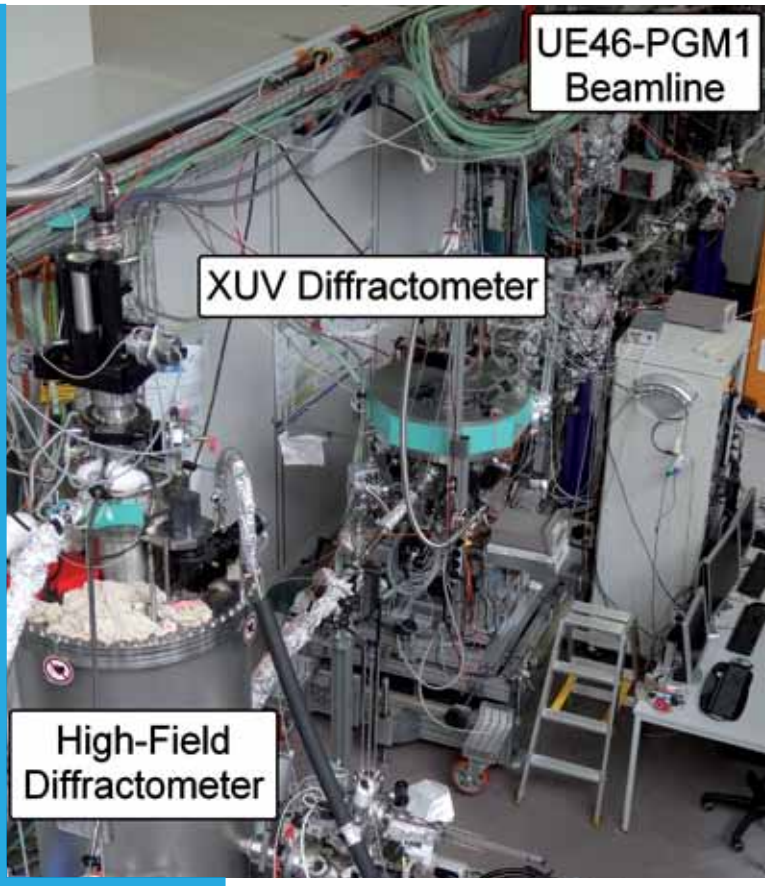
XM X-ray Microscopy - Reference guide for latest publications

UE46 PGM-1



UE46 PGM-1 is one of two beamlines situated at the elliptical undulator UE46. The beamline provides soft X-rays with tunable polarization (linear, circular) in the energy range between 120 eV and 2000 eV. It has a plane-grating design, the last mirror chamber hosts two mirrors that can be switched to provide a focussed or collimated beam. Techniques employed at UE46 PGM-1 include polarization-dependent X-ray absorption and resonant soft X-ray scattering experiments, covering a wide range of materials and scientific problems. Continuous-mode scanning is implemented at the beamline, a pair of energy-dependent X-ray absorption scans with opposite light helicities can be recorded with very high quality within less than 10 minutes. Depending on the sample, noise ratios as low as 10^{-4} can be achieved. The beamline hosts two permanent endstations, the XUV Diffractometer, an instrument dedicated to high performance RSXS studies and the High-Field Diffractometer, an instrument for RSXS and XAS studies in magnetic fields up to 7 Tesla. Both instruments can be used within the same beam time. Beamline and instruments are operated by the Department Quantum Phenomena in Novel Materials at HZB.

Instrument application

- Resonant diffraction from magnetic, charge, and orbital order superstructures
- Spectroscopy of electronic ordering phenomena
- Magnetization states of single molecular magnets
- Element-specific magnetic hysteresis loops
- Magnetization depth profiles

Instrument data

Location	11.2
Source	UE46
Monochromator	PGM
Energy range	120 - 2000 eV
Energy resolution	10000
Flux	10^{12}
Polarisation	• Linear any angle (with restrictions) • Circular
Divergence horizontal	1 mrad
Divergence vertical	1 mrad
Focus size (hor. x vert.)	• Focussed beam: typically 100 µm x 50 µm ultimate:40 µm x 10 µm • Collimated beam: ≤ 1.7 mm x 1.5 mm (depending on apertures)
Distance Focus/last valve	565 mm
Height Focus/floor level	1417 mm
Free photon beam available	Only under special conditions (please contact the beamline scientist before application)
Fixed end station	Yes
Instrument responsible	Dr. Eugen Weschke, eugen.weschke@helmholtz-berlin.de Dr. Enrico Schierle, enrico.schierle@helmholtz-berlin.de

References / Latest publications

[1] Ghiringhelli, G. *et al.*: Long-Range Incommensurate Charge Fluctuations in (Y,Nd)$Ba_2Cu_3O_{6+x}$, Science 337 (2012), 821.

[2] Blanco-Canosa, S. *et al.*: Momentum-Dependent Charge Correlations in $YBa_2Cu_3O_{6-d}$ Superconductors Probed by Resonant X-ray Scattering: Evidence for Three Competing Phases, Phys. Rev. Lett. 110 (2013), 187001.

[3] Schmitz-Antoniak, C. *et al.*: Electric In-Plane Polarization in Multiferroic $CoFe_2O_4$ / $BaTiO_3$ Nanocomposite Tuned by Magnetic Fields, Nature Communications 4 (2013), 2051.

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

UE46 PGM-1 - Reference guide for latest publications

High-Field Diffractometer

The High-Field Diffractometer is an endstation for both soft-X-ray absorption (XAS) and resonant soft X-ray scattering (RSXS) in magnetic fields up to 7 Tesla and temperatures down to 4 K. This combination of high magnetic fields and low temperatures renders the setup ideal for studying weakly coupled magnetic systems like diluted magnets or single molecular magnets. The unique feature of this endstation is an in-vacuum superconducting coil that can be rotated independently from the sample. The station is therefore perfectly suited for XMCD and XMLD experiments in various geometries. The absorption signal is typically measured in the TEY-mode via the sample drain current. Employing continuous mode, a pair of energy-dependent absorption scans with opposite light helicities can be recorded with very high quality within less than 10 minutes. Depending on the sample, noise ratios as low as 10^{-4} can be achieved. A rotatable photon detector enables to perform dichroism experiments using specular reflectivity, which is often more sensitive to tiny magnetizations at interfaces and less surface sensitive than TEY-mode experiments. The same detector permits RSXS experiments at relevant scattering geometries to study the evolution of electronic ordering phenomena, like charge and orbital ordering in high magnetic fields, being at the heart of many of todays most fascinating macroscopic phenomena in complex oxides.

Samples are transferred in a fast and reliable way from outside vacuum to a sample holder directly attached to a LHe-flow cryostat

that provides the base temperatures of 4 K. The endstation is permanently attached to the UE46 PGM-1 beamline providing high photon flux between 120 eV and 2000 eV and variable photon polarization. The beamline also hosts the XUV Diffractometer, an instrument dedicated to high performance RSXS studies. Both instruments can be used within the same beam time. Beamline and instruments are operated by the Department Quantum Phenomena in Novel Materials at HZB.

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

Instrument data

Monochromator	PGM
Experiment in vacuum	Yes
Temperature range	4 - 35 K
Detector	AXUV100 type photodiode
Magnetic Field	Standard: 6 Tesla (for fields up to 7 Tesla contact Station Managers)
Magnetic Field Geometry	Horizontal, rotatable (90 deg.) with respect to sample
Scattering Geometry	Horizontal
Sample rotation	0 deg. to 90 deg. with respect to the photon beam
Scattering angles	Limited, depending on orientation of the magnet
Software	SPEC
Instrument responsible	Dr. Eugen Weschke, eugen.weschke@helmholtz-berlin.de Dr. E. Schierle, enrico.schierle@helmholtz-berlin.de

Instrument application

- Diffraction from complex electronic superstructures (magnetic, charge and orbital order)
- Magnetization states of single molecular magnets
- Element-specific magnetic hysteresis loops (switching behavior in heterostructures or alloys, exchange bias)
- Electronic ground states in crystals

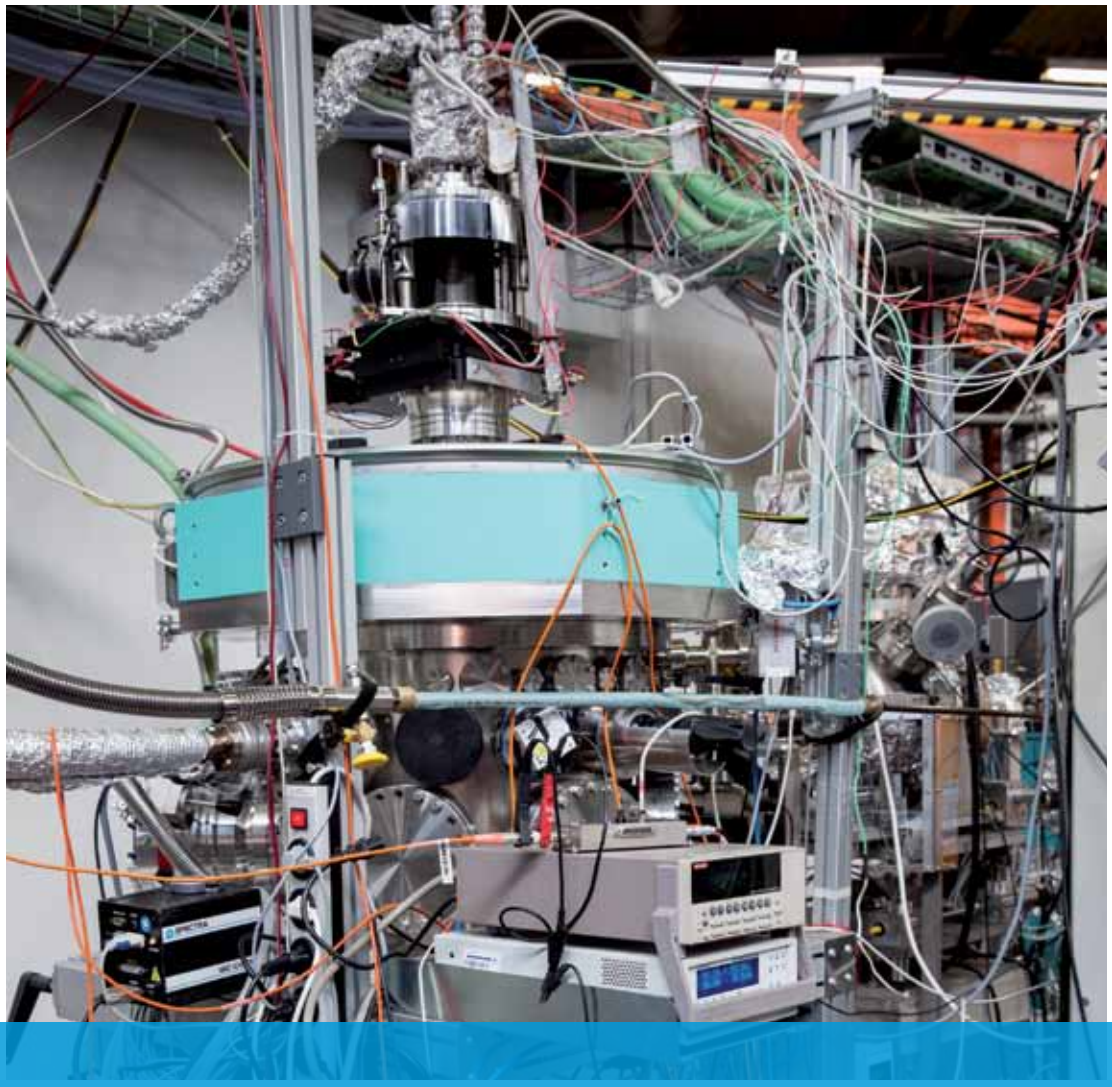
High-Field Diffractometer - Reference guide for latest publications

References / Latest publications

[1] Blanco-Canosa, S. *et al.*: Momentum-Dependent Charge Correlations in $YBa_2Cu_3O_{6-d}$ Superconductors Probed by Resonant X-ray Scattering: Evidence for Three Competing Phases, Phys. Rev. Lett. 110 (2013), 187001.

[2] Hermanns, C. *et al.*: Magnetic Coupling of $Gd_3N@C_{80}$ Endohedral Fullerenes to a Substrate, Phys. Rev. Lett. 111 (2013), 167203.

[3] Schmitz-Antoniak, C. *et al.*: Electric In-Plane Polarisation in Multiferroic $CoFe_2O_4$ / $BaTiO_3$ Nanocomposite Tuned by Magnetic Fields, Nature Communications 4 (2013), 2051.



XUV Diffractometer
for Resonant Soft X-ray Scattering

The XUV Diffractometer is a dedicated endstation to explore electronic ordering phenomena, like magnetic, charge and orbital ordering by resonant soft X-ray scattering (RSXS) experiments. This versatile endstation is a UHV-compatible two-circle diffractometer operating in horizontal scattering geometry with the sample and detector rotations driven from outside vacuum by Huber circles with highest accuracy and stability. It allows to perform high quality diffraction experiments even from tiny crystals (< 100 µm x 100 µm) over a large angular range as well as measurements of specular reflectivity with very high accuracy. With the samples mounted directly to a LHe-flow-cryostat, sample temperatures below 4 K can be reached. Azimuthal rotation *in-situ* is provided for azimuth-dependent

measurements. Photons are detected by an AXUV100-type photodiode with a set of changeable slits in front for optimizing the q-resolution. The detector can be scanned in the direction perpendicular to the scattering plane. This allows to compensate possible Chi-misalignment without compromising about the lowest sample temperatures. The experimental setup allows for X-ray absorption (XAS) measurements by parallel monitoring of the sample drain current (TEY measurements) as well as for FY measurements. The instrument is flexible and can adapt to special sample mounting. The endstation is permanently attached to the UE46 PGM-1 beamline providing high photon flux between 120 eV and 2000 eV and variable photon polarization. The beamline also hosts the High-Field Diffractometer, an instrument for RSXS and XAS studies in magnetic fields up to 7 Tesla. Both instruments can be used within the same beam time. Beamline and instruments are operated by the Department Quantum Phenomena in Novel Materials at HZB.

Instrument data

Monochromator	PGM
Experiment in vacuum	Yes
Temperature range	3.8 - 320 K (for T = 3.0 K contact Station Managers)
Detector	AXUV100 type photodiode
Scattering Geometry	Horizontal
Angular range	Unlimited (360 deg.)
maximum sample size	5 mm x 5 mm
azimuthal sample rotation	Yes
Software	SPEC
Instrument responsible	Dr. Eugen Weschke, eugen.weschke@helmholtz-berlin.de Dr. Enrico Schierle, enrico.schierle@helmholtz-berlin.de

Instrument application

- Diffraction from complex electronic ordering phenomena (magnetic, charge and orbital order)
- Interfacial electronic properties in heterostructures
- Magnetic structure determination even from tiny single crystals and nanostructures
- Magnetization depth profiles

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

References / Latest publications

[1] Fink, J. *et al.*: Resonant Elastic Soft X-ray Scattering, Report on Progress in Physics 76 (2013), 056502.

[2] Frano, A. *et al.*: Orbital Control of Noncollinear Magnetic Order in Nickel Oxide Heterostructures, Phys. Rev. Lett. 111 (2013), 106804.

[3] Ghiringhelli, G. *et al.*: Long-Range Incommensurate Charge Fluctuations in (Y,Nd)$Ba_2Cu_3O_{6+x}$, Science 337 (2012), 821.

XUV Diff - Reference guide for latest publications

Instrument application

RIXS:

- Study of low-energy excitations in solids (study of magnetic, orbital, nuclear and charge degrees of freedom and their interplay)
- Study of the electronic structure of solids (the size of band-gaps and band-widths)
- Study of materials showing phase separation with µm-real-space resolution

CXS:

- X-ray holography, coherent diffraction imaging and ptychography
- Coherent resonant X-ray scattering in transmission and reflection geometry
- Nanomagnetism

UE49 SGM

The RICXS beamline is a dedicated beamline, which accomodates two permanent experimental set-ups for X-ray scattering: the Resonant Inelastic X-ray Scattering (RIXS) and the Coherent X-ray Scattering (CXS) end-stations.

The RIXS experiment is designed for resonant X-ray Raman studies of solid samples under ultra-high vacuum conditions and in the temperature range from liquid-He to room temperature. It is equipped with a confocal plane grating spectrometer, which allows optimising the operation mode between high signal-transmission and high energy-resolution.

The CXS set-up allows the use of coherent X-rays in scattering and imaging applications. In particular, the transverse and longitudinal coherence length can be optimized for the particular experiment to maximize the coherent photon flux on the sample. A large part of reciprocal space can be covered by a moveable 2048 x 2048 pixel soft X-ray CCD detector (moveable by ±45° horizontally and vertically with adjustable oversampling ratio). A 3D magnetic vector field of up to 1T is available as sample environment.

The characteristics of the RICXS beamline were designed to meet the high demands of the two techniques, which are high (coherent) photon flux, a µm-size beam focus and full polarization control (linear and circular). It can be operated in the energy range 95 – 1400 eV, covering the resonant transitions of many relevant elements, such as silicon and phosphor L-edges, lanthanide N4,5-

edges, carbon, nitrogen and oxygen K-edges, transition metal L2,3-edges. The beamline is realized as a spherical grating monochromator (SGM) with a Kirkpatrick Baez refocusing stage. The monochromator accomodates three laminar gratings: 180 l/mm (operation range: 95 – 270 eV, best energy resolving power E/ΔE = 6500 at 95 eV), 410 l/mm (180 – 650 eV, E/ΔE = 10000 at 210 eV), 900 l/mm (400 – 1400 eV, E/ΔE = 12000 at 450 eV).

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

Instrument data

Location	10.1
Source	UE49
Monochromator	Spherical VLS grating monochromator
Energy range	90 - 1400 eV
Energy resolution	4000 - 12000
Flux	Up to $7 \cdot 10^{14}$ photons / s / 0.1A / 0.1%BW
Polarisation	Full polarization control
Focus size (hor. x vert.)	4 µm x 1 µm (hor. x vert.)
Height Focus/floor level	1100 mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Annette Pietzsch, annette.pietzsch@helmholtz-berlin.de Dr. Justine Schlappa, justine.schlappa@helmholtz-berlin.de

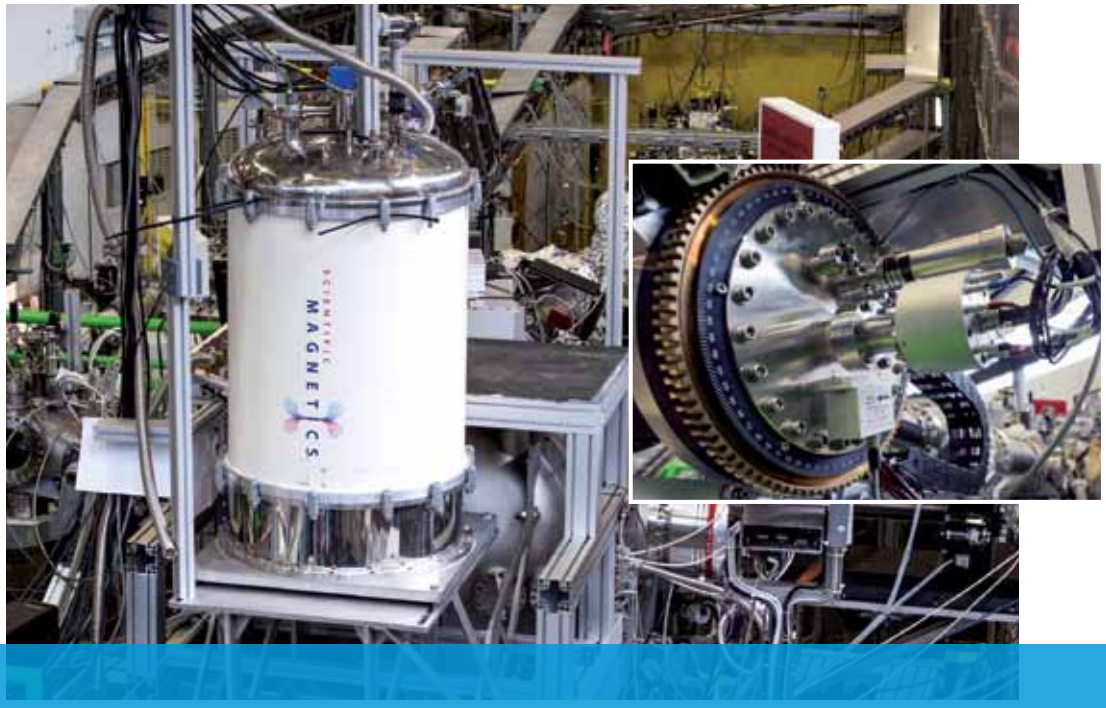
References / Latest publications

[1] Ewerlin, M. *et al.*: Magnetic Dipole and Higher Pole Interaction on a Square Lattice, Phys. Rev. Lett. 110 (2013), 177209.

[2] Bali, R. *et al.*: Printing Nearly-Discrete Magnetic Patterns Using Chemical Disorder Induced Ferromagnetism, Nano Letters 14 (2014), 435-441.

[3] Cherifi, R.O. *et al.*: Electric-field control of magnetic order above room temperature, Nature Materials 13 (2014), 345-351.

UE49 SGM - Reference guide for latest publications



µmRIXS

The µmRIXS plane grating spectrometer consists of two parabolical mirrors with a plane grating in between. The first mirror collects and collimates the radiation from the 1x4 µm² beamline microfocus on the sample onto the grating while the second mirror focusses the diffracted light onto the detector. The spectrometer houses two laminar grating structures on a common substrate: 1050 l/mm for high transmission and 4200 l/mm for high resolution. The photons are detected by a PHOTONIS multi channel pate (MCP) stack in combination with a RoentDek delay line detector DLD-120. The MCP channel diameter is 25 µm and the top MCP is coated with CsI to improve the quantum efficiency of the detektor.

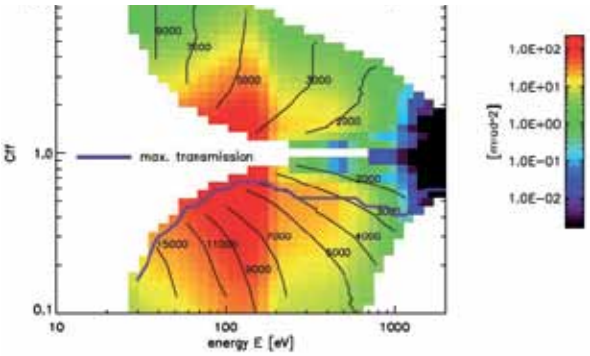
The samples are mounted in the solid state experimental chamber directly to a Janis ST-500 Microscopy Cryostate which allows for a maximum stability for the sample position. To avoid mechanical instabilities in sample positioning, no sample translation stage is installed, but the whole vacuum chamber can be positioned by a 3-axis Huber table vertically and in the horizontal plane. Rotation of the sample around the vertical axis is achieved via a rotation of the microscope cryostate.

The µmRIXS spectrometer is permanently situated at the UE49-SGM beamline while the solid state experimental chamber can be exchanged for the coherent X-ray scattering (CXS) chamber.

Instrument data

Energy range	Soft X-rays from 90 to around 1000 eV, resolving power better than 2000
Sample environment	Solid samples in vacuum, sample transfer
Temperature range	From liquid helium temperatures to 600 K
Detectors	Plane grating spectrometer with MCP stack + Delay line detector, GaAs photodiode
Manipulators	He cryostate with 4 degrees of freedom, all motorized
Instrument responsible	Dr. Justine Schlappa, justine.schlappa@helmholtz-berlin.de

Spectrometer resolution/transmission.



(a) The 1050 $\frac{l}{mm}$ grating structure.

Instrument application

- RIXS with micrometer focus on solid samples
- Fluorescence yield absorption spectroscopy with micrometer focus
- Temperature dependent measurements

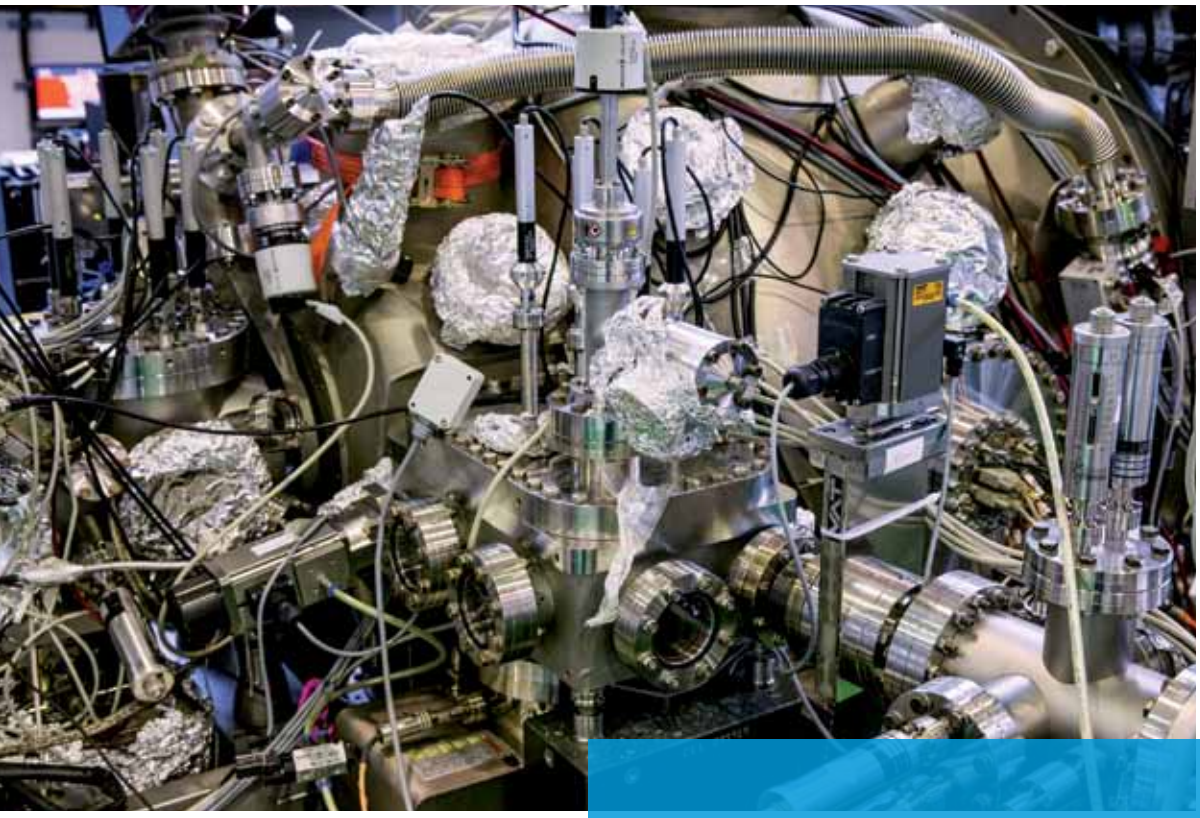
EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

References / Latest publications

Könnecke, R. *et al.*: The confocal plane grating spectrometer at BESSY II, J. Electron Relat. Phenom. 188 (2013), 133-139.

RIXS - Reference guide for latest publications



EXPERIMENTAL
HALL BESSY II

FIXED STATIONS
CRG BESSY II

Instrument application

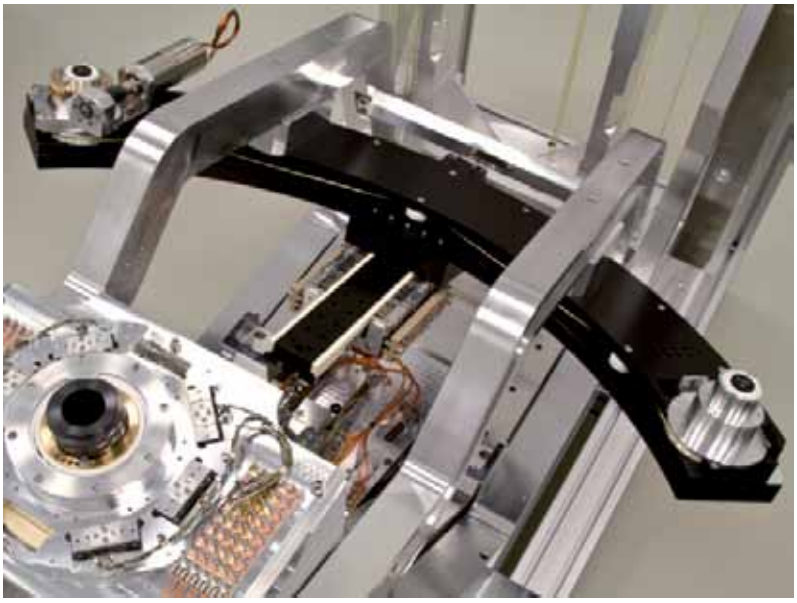
- Nanomagnetism
- Thin magnetic films and multilayers
- Magnetization dynamics (pump-probe)
- Interference based imaging approaches
- Nanoscale imaging incl. spectro-microscopy
- Nanostructured materials

CXS | Coherent X-ray Scattering

The coherent X-ray scattering (CXS) endstation at UE49 SGM allows utilizing the high coherent photon flux from a BESSY II low-beta undulator for X-ray interference based experiments. The setup is very flexible in its scattering geometry via an in vacuum movable CCD detector, allowing for experiments in both transmission and reflection. Also due to the few optical element beamline design, the coherent flux is exceptionally high and coherence parameters of the illumination can be adjusted *in-situ*. X-ray magnetic dichroism can be used for spectroscopic, scattering or imaging contrast via the availability of a 1T magnetic field at the sample and full polarization control of the soft X-ray beam.

Instrument data

Sample	• Size: 2 x 2 mm^2 up to 10 x 10 mm^2 • Standard sample holder with 16 electrical contacts.
Sample nanomanipulator	x,y,z,(±5 mm with 100 nm resolution) and 180° rotation allowing for experiments in transmission and reflection geometry.
Magnetic field @ sample	≤ 1 Tesla 3D vector
Coherent illumination	Coherent photon flux vs. transverse coherence tradable *in-situ*
Focus	1x4µm KB-focus of UE49 SGM beamline, full polarization control, fed from L08 low-beta section of BESSY II
Detector	Back-illuminated soft X-ray CCD 2048 x 2048 pixel with 13.5 µm pixel size. *In-situ* adjustable central beamstop.
reciprocal space flexibility	Sample-CCD distance: 250 - 450 mm allowing to vary field of view and oversampling ratio, rotation of CCD by ±20° around the sample both horizontally and vertically
Standard experiments	Coherent scattering and coherent diffraction imaging, Fourier transform holography, ptychography, all in X-ray dichroic and resonant (magnetic) scattering variants.
Instrument responsible	Dr. Wolfgang-Dietrich Engel, dietrich.engel@helmholtz-berlin.de



CXS- Reference guide for latest publications

SPEEM | Spin resolved Photoemission Microscope

Magnetic nanostructures are at the heart of modern data storage technology. Typical dimensions of magnetic bits are in the sub-100nm region. In addition novel magneto-electronics devices such as magnetic random access memory junctions are operated on the sub-100 nm m scale. An understanding magnetic properties of such low-dimensional structures is only accessible to spectro-microscopy tools capable of appropriate lateral resolution. This goal is achieved by combining a photoemission microscope (SPEEM) with a dedicated microfocus PGM beamline (UE49 PGM). High photon flux in combination with full polarization control makes this setup the ideal tool for space resolved and element selective investigation of nanostructures by means of chemical maps (XAS) and magnetic imaging (XMCD and XLD).

Instrument data

SPEEM Microscope	
Spatial resolution	25 nm
Energy analyzer	DE < 0.3 eV
Monochromator	PGM
Azimuth rotation	Yes
Temperatur control	65 K - 600 K
Electic and magnetic field	max. 75 mT during imaging
Beamline	
Monochromator	PGM
Energy range	80 to 1800 eV
Energy resolution	10.000 at 700 eV
Spot size on sample	10 x 20 µm
Full polarization control	Yes
Fixed endstation	Yes
Preparation chamber	• Evaporation Fe, Co, Ni, Al... • Ion sputtering • Sample storage in vacuum up to 6
Pump Laser	• 800 nm wavelength • 300 nJ max. pulse energy • 80 fs pulse duration • Repetition rate variable from single pulse to 2.5 MHz
Instrument responsible	Dr. Florian Kronast, florian.kronast@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

FIXED STATIONS BESSY II

SPEEM - Reference guide for latest publications

Instrument application

- Chemical maps by XAS and XPS
- Magnetic domain imaging by XMCD and XMLD
- Micro-spectroscopy on nanostructures, magnetic responses and interactions, probing of core shell structures
- Magnetic transport and spin torque
- Magnetic/magnetoelectric coupling in thin films and multifoerroics
- Time-resolved magnetization dynamics (fs-laser pump, X-ray probe)

References / Latest publications

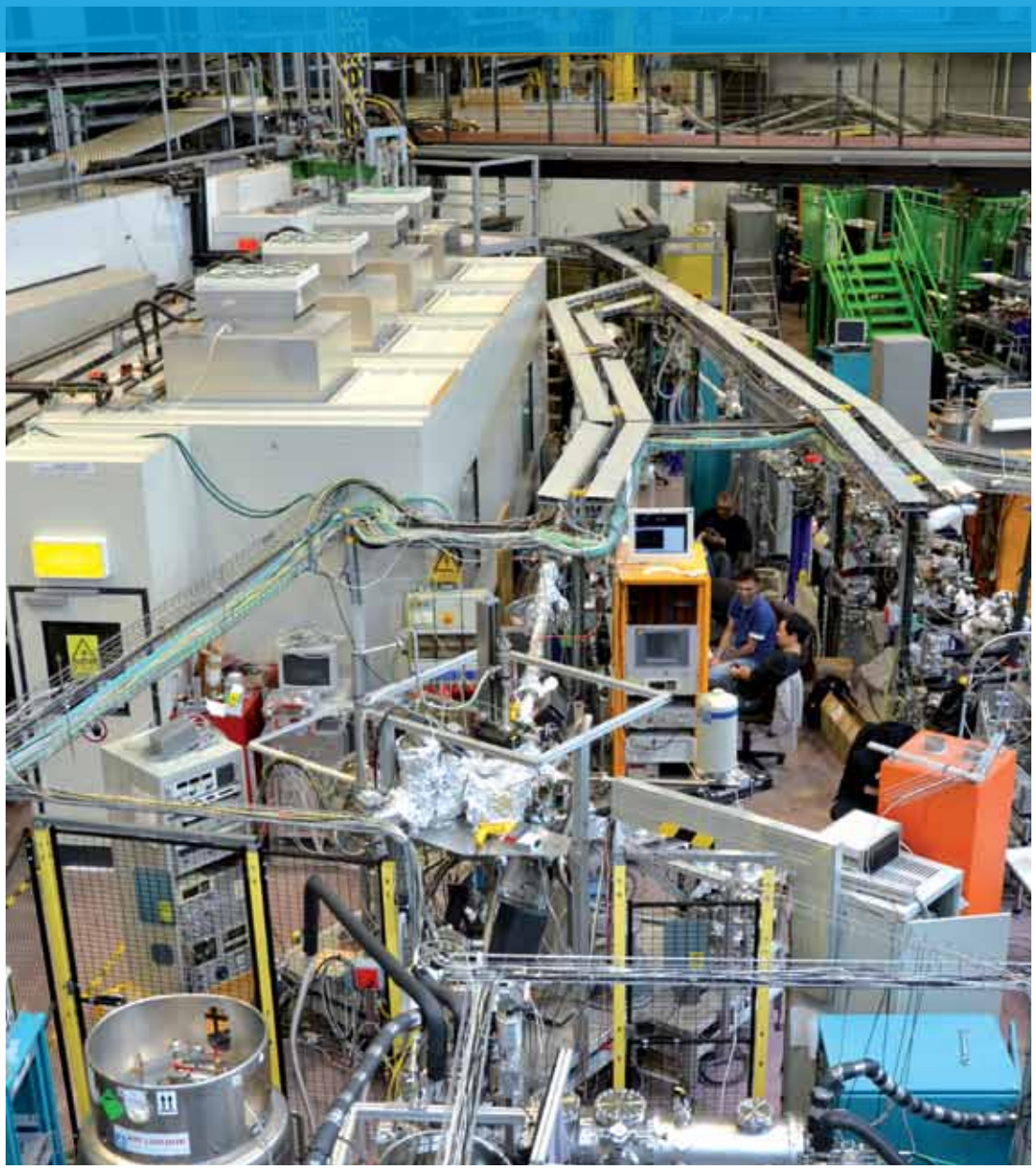
[1] Ewerlin, M. *et al.*: Magnetic Dipole and Higher Pole Interaction on a Square Lattice, Phys. Rev. Lett. 110 (2013), 177209.

[2] Bali, R. *et al.*: Printing Nearly-Discrete Magnetic Patterns Using Chemical Disorder Induced Ferromagnetism, Nano Letters 14 (2014), 435-441.

[3] Cherifi, R.O. *et al.*: Electric-field control of magnetic order above room temperature, Nature Materials 13 (2014), 345-351.

UE52 PGM

Variable polarization undulator beamline with plane-grating monochromator. This beamline currently hosts the UE52 PGM-PES end station, but can also be used to setup experimental stations in the free-port section. The HZB Nanocluster trap endstation is frequently installed at UE52 PGM.



Instrument data

Location	10.2
Source	UE52
Monochromator	PGM
Energy range	85 - 1600 eV
Energy resolution	> 10000 at 400 eV
Flux	10^{12}
Polarisation	Variable
Divergence horizontal	0.8 mrad
Divergence vertical	0.2 mrad
Distance Focus/last valve	1000 mm
Height Focus/floor level	1412 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Tobias Lau, tobias.lau@helmholtz-berlin.de Dr. Arkadiusz Lawicki, arkadiusz.lawicki@helmholtz-berlin.de

Instrument application

Beamline UE52 PGM is used to investigate magnetic and electronic properties of a large variety of different samples. This beamline hosts a permanent photoemission endstation with a Scienta 4000 analyzer and is currently upgraded to additional ARToF analyzers for coincidence spectroscopy. Because of its beam characteristics, UE52 PGM also frequently hosts the Nanocluster Trap endstation, which can be setup out-of-focus behind the photoemission experiment.

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

References / Latest publications

[1] Zamudio-Bayer, V. *et al.*: Coordination-driven magnetic-to-nonmagnetic transition in manganese doped silicon clusters, Phys. Rev. B 88 (2013), 115425.

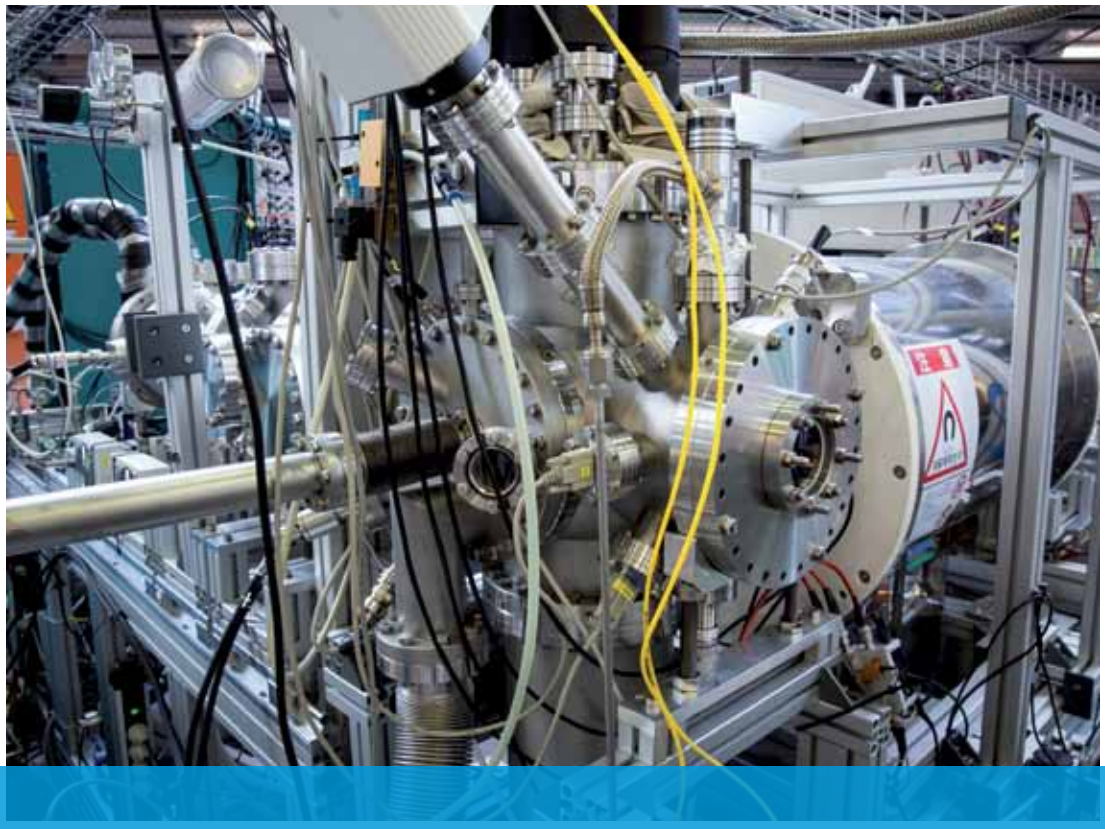
[2] Niemeyer, M. *et al.*: Spin coupling and orbital angular momentum in free iron clusters, Phys. Rev. Lett. 108 (2012), 057201.

[3] Eralp, T. *et al.*: The Importance of Attractive Three-Point Interaction in Enantioselective Surface Chemistry: Stereospecific Adsorption of Serine on the Intrinsically Chiral Cu{531} Surface, J. Am. Chem. Soc. 134 (2012), 9615-9621.

[4] Usachov, D. *et al.*: Nitrogen-Doped Graphene: Efficient Growth, Structure, and Electronic Properties, Nano Lett. 11 (2011), 5401-5407.

[5] Wlodarczyk, R. *et al.*: Tuning the electronic structure of ultrathin crystalline silica films on Ru(0001), Phys. Rev. B 85 (2012), 085403.

UE52 PGM - Reference guide for latest publications



NanoclusterTrap

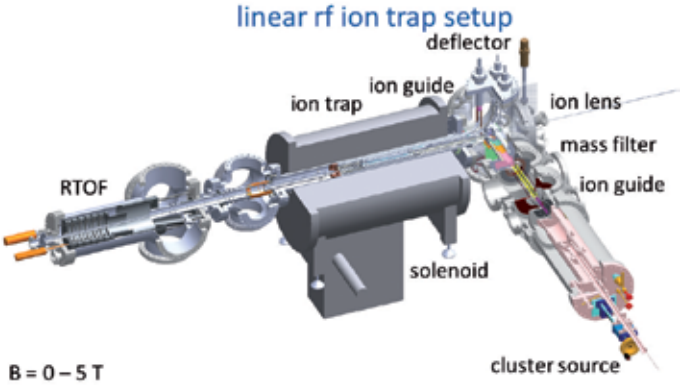
Cryogenic linear quadrupole ion trap with 5 T superconducting solenoid for X-ray magnetic linear dichroism spectroscopy of size-selected clusters, molecular ions, and complexes. Because of its complexity, this experiment requires thorough consultation with the scientist in charge. Please contact us well ahead of time to discuss experimental feasibility. Nanocluster trap is jointly operated by Helmholtz-Zentrum Berlin, Uni Freiburg, TU Berlin, Kyushu University, and Toyota Technological Institute.

Instrument application

The Nanocluster Trap instrument at BESSY II is used to investigate magnetic phenomena on the atomic scale. Often used in combination with a magnetron cluster source, magnetic spin and orbital moments of size-selected pure and mixed transition metal clusters, molecules, and complexes can be determined. The ion trap can also be combined with a variety of ion sources (*e.g.*, electrospray ionization or laser evaporation) because of a flexible interface to the first ion guide.
Nanocluster Trap is currently being upgraded to even more flexible ion trapping schemes and even lower cryogenic (T < 5 K) ion temperature within BMBF project 05K13Vf2 hosted at Universität Freiburg.

Instrument data

Experiment in vacuum	Yes
Temperature range	5 - 300 K
Detector	High transmission reflectron time-of-flight mass spectrometer for ion yield spectroscpy
Manipulators	Cryogenic linear quadrupole ion trap
Applied magnetic field	0 - 5 T
Mass range	10 - 4000 amu
Circularly polarized radiation	Yes
Instrument responsible	Dr. Tobias Lau, tobias.lau@helmholtz-berlin.de Dr. Arkadiusz Lawicki, arkadiusz.lawicki@helmholtz-berlin.de



B = 0 – 5 T
T < 10 K (He buffer gas, **thermal equilibrium**)
$\rho = 5 \times 10^7$ ions cm^{-3}
$\Phi = 10^{12}$ ph s^{-1}
BESSY II UE52-SGM/PGM

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

References / Latest publications

[1] Zamudio-Bayer, V. *et al.*: Coordination-driven magnetic-to-nonmagnetic transition in manganese doped silicon clusters, Phys. Rev. B 88 (2013), 115425.

[2] Niemeyer, M. *et al.*: Spin coupling and orbital angular momentum in free iron clusters, Phys. Rev. Lett. 108 (2012), 057201.

[3] Hirsch K. *et al.*: 2p X-ray absorption of free transition metal cations across the 3d transition elements: calcium through copper, Phys. Rev. A 85 (2012), 062501.

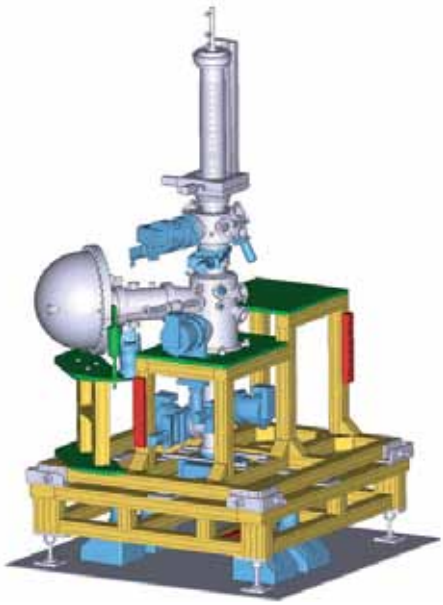
NanoclusterTrap - Reference guide for latest publications

One-squared ARPES | 1^2-ARPES ultra high resolution photoemission station

The 1^2 angle-resolved photoemission station is the more versatile sibling of the low-temperature 1^3 end-station. While it receives light from the same beam-line and is equipped with a very high resolution electron energy analyzer, it sheds the ability to reach the lowest temperatures in favor of a much more flexible 6 axes manipulator.
The versatility of the system is furthered by two sample handling options: it can be either be used with Cu sample holders for low temperature applications or Omicron sample plates for enhanced sample preparation flexibility. The system is permanently attached to the UE112 PGM-2a beamline (Location 14.2) which can provide photons in the energy range from 10-250 eV with very high resolution and full control over the polarization.

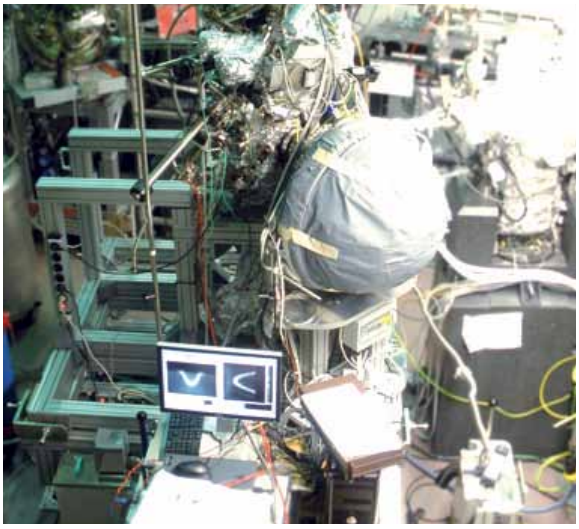
Instrument application

- High-resolution angle-resolved photoelectron spectroscopy.
- Low energy electron diffraction
- Preparative sample heating up to 2300 K
- Quadrupole mass spectrometer
- e-Beam evaporators



Instrument data

Monochromator	Low energy collimated plane-grating monochromator with normal incidence option
Experiment in vacuum	Yes
Temperature range	Measurement: 20–400 K; Preparation up to 2300 K
Detector	Scienta R8000
Manipulators	Motorized 6 axes manipulator (IFW Dresden design)
Instrument responsible	Dr. Andrei Varykhalov, andrei.varykhalov@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

FIXED STATIONS BESSY II

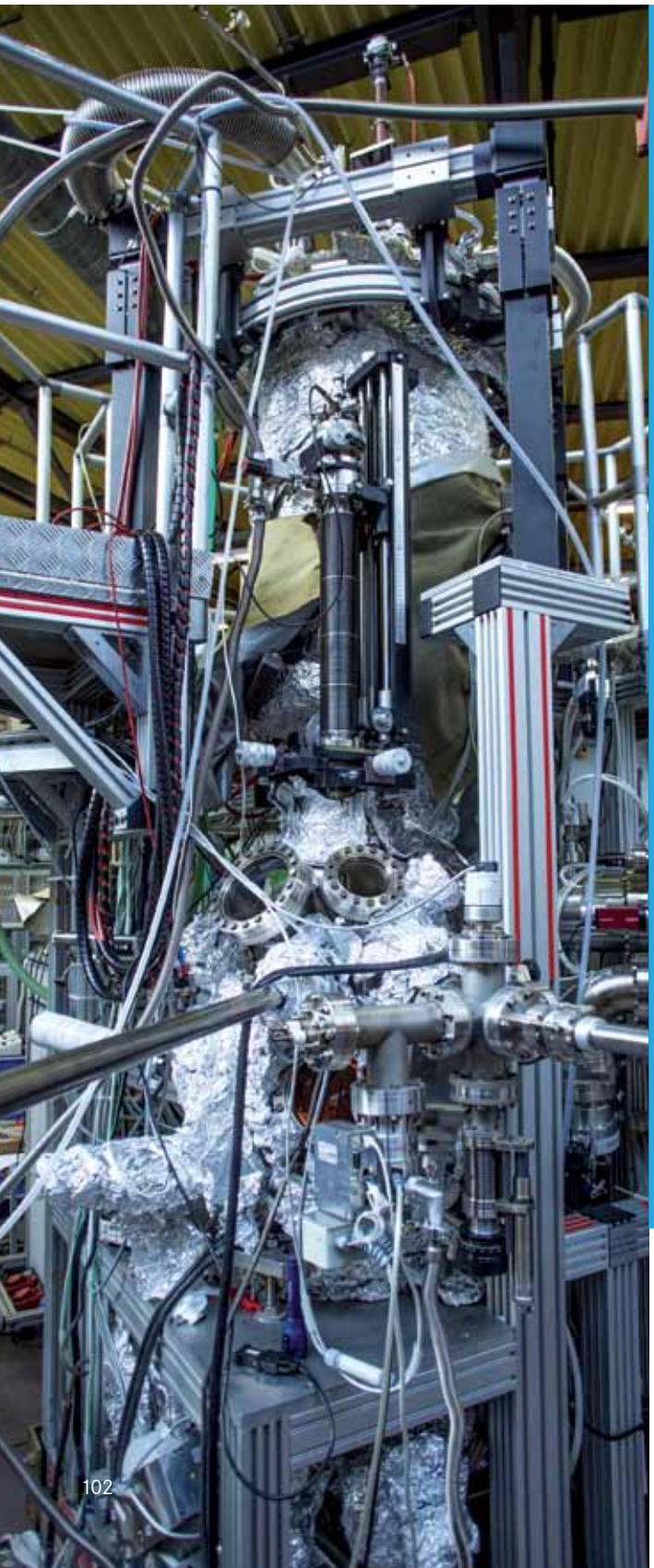
References / Latest publications

[1] Frantzeskakis, E., *et al.*: Kondo Hybridization and the Origin of Metallic States at the (001) Surface of SmB_6, Physical Review X 3 (2013), 041024.

[2] Scholz, M.R. *et al.*: Reversal of the Circular Dichroism in Angle-Resolved Photoemission from Bi_2Te_3, Physical Review Letters 110 (2013), 216801.

[3] Pauly, Ch. *et al.*: Evidence for topological band inversion of the phase change material $Ge_2Sb_2Te_6$, Applied Physics Letters 103 (2013), 243109.

One-squared ARPES - Reference guide for latest publications



1^3 **ARPES** | Ultra high resolution photoemission station

The station is designed for angle-resolved photoelectron spectroscopy at the highest energy resolution and ultimately low sample temperatures. In this system, all contributors to experimental broadening –the resolution of both the excitation source and the electron energy analyzer as well as the sample temperature– have been reduced to 1 meV or their equivalent, yielding the name of the station: 1 meV x 1 meV x 1 K = 1^3.

A purpose-built ^{3}He cryostat forms the heart of the system and allows for sample temperatures down to 1 K. To provide the required thermal anchoring, only the polar angle of the sample can be changed during measurement. The azimuthal angle of the sample can, however, be adjusted by means of the sample transfer mechanism. The entrance slit of the analyzer is mounted parallel to the polar rotation axis which allows for Fermi surface mapping. The system is permanently attached to the UE112 PGM2 beamline which can provide photons in the energy range from 5-250 eV with very high resolution and full control over the polarization.

Instrument application

- High resolution studies on the electronic structure of materials with very low critical temperatures such as heavy-Fermion and quantum critical systems.
- Determination of the 3-D gap structure of novel high-T_c superconductors.

Instrument data

Monochromator	Low energy plane grating monochromator with normal incidence option
Source	UE112
Energy range	5 - 250 eV
Energy resolution	< 1 meV for E < 100 eV
Polarization	Linear any angle, circular
Divergence horizontal	1 mrad
Divergence vertical	3 mrad
Free photon beam available	No
Fixed end station	Yes
Experiment in vacuum	Yes
Temperature range	1 - 50 K
Detector	Scienta R4000 Electron Spectrometer
Manipulators	^{3}He Cryomanipulator with 3 translational and one rotational degree of freedom
Sample characterization	4-grid LEED optics
Instrument responsible	Dr. Emile Rienks, emile.rienks@helmholtz-berlin.de

References / Latest publications

[1] Ge, Q. Q. *et al.*: Anisotropic but Nodeless Superconducting Gap in the Presence of Spin-Density Wave in Iron-Pnictide Superconductor $NaFe_{1-x}Co_xAs$, Phys. Rev. X 3 (2013), 011020.

[2] Boariu, F. L. *et al.*: Momentum-Resolved Evolution of the Kondo Lattice into 'Hidden Order' in URu_2Si_2, Phys. Rev. Lett. 110 (2013), 156404.

[3] Chatterjee, S. *et al.*: Formation of the Coherent Heavy Fermion Liquid at the Hidden Order Transition in URu_2Si_2, Phys. Rev. Lett. 110 (2013), 186401.

EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

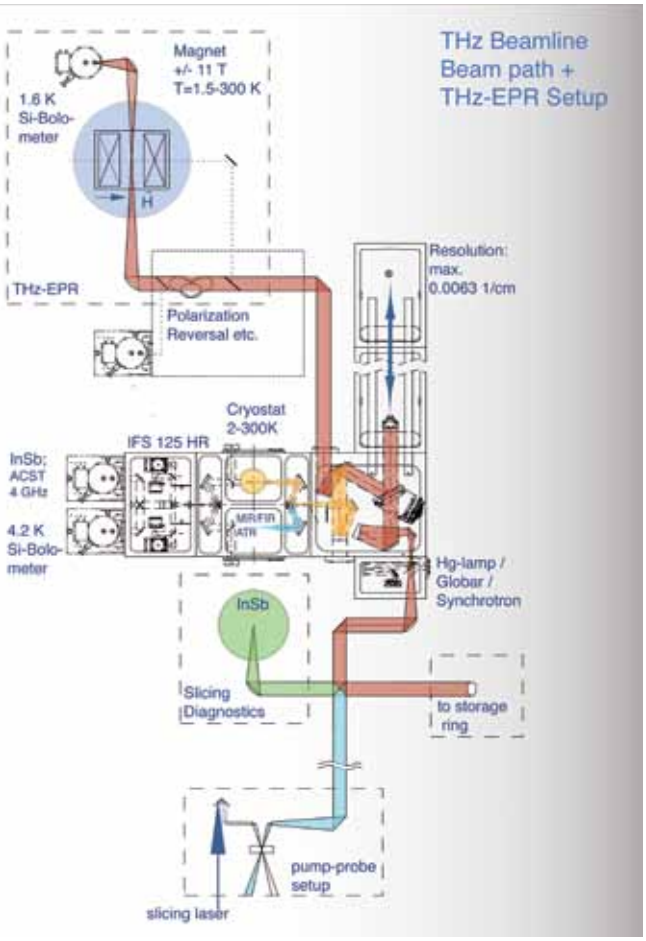
FIXED STATIONS BESSY II

1^3 ARPES - Reference guide for latest publications

THz Beamline

The THz beamline exploits intense coherent synchrotron radiation (CSR) as emitted from special storage ring modes, for the study of magneto optical phenomena in the energy range from 3 to 150 cm^{-1}. A dedicated THz electron paramagnetic resonance (THz-EPR) facility combines a broad range of excitation and detection schemes with extreme sample environments (in particular high magnetic fields and low temperatures). Research topics are related to manipulation and detection of high spin states in *e.g.*, proteins, single molecule magnets, energy materials and materials relevant for future information technologies.

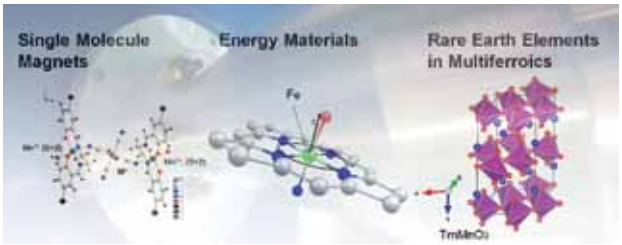
The THz beamline extracts CSR from the 2° dipole source (D112) after the slicing section at an acceptance of 60 mrad (h) x 15 mrad (v). A true optical transmission line transports CSR as emitted by ultra-short bunches in the low a mode (pulse length: < 10 ps, spectral range: 3-50 cm^{-1}) [1] and laser-induced by femtoslicing [2] (pulse length: ~ 200 fs, spectral range: 20-150 cm^{-1}), respectively. Complementary, FIR-UV-VIS cw radiation and 1 mJ of synchronized fs laser pulses (800 or 400 nm) are available at the experiment. Sample environments include a superconducting



magnet (Oxford Spectromag, -11 T to +11 T) equipped with a variable temperature insert (1.5 - 200 K), and an optical cryostat (Oxford Optistat, T = 1.5 - 300 K). THz detection is achieved either with a high resolution FTIR-spectrometer (Bruker IFS 125-HR, min. bandwidth: 0.0063 cm^{-1}) in combination with ultra-sensitive liquid helium cooled Si- or InSb – bolometers or fast Schottky diode THz detectors (ACST, time resolution 250 ps). Alternatively, transient THz signals may be directly detected via a time domain (TD) THz set-up. This dedicated TD THz scheme allows for a cross-correlation of THz pulses from the storage ring with the synchronized external fs-laser source (optical pump – THz probe).

Instrument data

Location	12.1
Source	D112
Monochromator	FTIR-Spectrometer IFS125 HR (Bruker Optics) and VERTEX 70
Energy range	5 1/cm 10000 1/cm
Energy resolution	0.0063 1/cm
Flux	5 mW/mm²
Polarization	Variable
Divergence horizontal	60 mrad
Divergence vertical	15 mrad
Focus size (hor. x vert.)	> 0.3 x 0.3 mm
Distance Focus/last valve	900 mm
Height Focus/floor level	1200 mm
Free photon beam available	Yes
Fixed end station	Yes
Instrument responsible	Dr. Karsten Holldack, karsten.holldack@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES BESSY II

Instrument application

Main science drivers are investigations in spin coupling energies of high spin transition metal and rare earth ions. Spin coupling energies are sensitive probes of the electronic structure and determine magnetic properties of compounds with unpaired electron spins. The latter are highly desired pieces of information, as high spin paramagnetic ions determine the function of many vital catalytic processes in proteins and synthetic complexes, as well as the properties of systems with large exchange couplings, *e.g.* single molecule magnets, energy materials or . The ideal technique to explore magnetic structure-function relationships of materials containing unpaired electron spins is EPR. However, conventional single frequency EPR frequently fails in cases where spin transition energies exceed the quantum energy of the spectrometer (typically < 4 cm^{-1}). Recently, we have demonstrated that CSR based FD-FT THz-EPR [3] provides a unique tool to overcome this restriction. Our novel approach allows for EPR excitations over a broad energy (3 cm^{-1} – 150 cm^{-1}) and magnetic field range (-11 T - +11 T) in a single spectrometer. FD-FT THz-EPR has been successfully applied to high spin ions in single molecule magnets [4, 5] catalytic mononuclear integer HS TMI complexes and very recently even in proteins and in strongly correlated solid state systems.

References / Latest publications

[1] Abo-Bakr, M. *et al.*: Brilliant, Coherent Far-Infrared (THz) Synchrotron Radiation, Phys. Rev. Lett. 90 (2003), 094801.

[2] Holldack, K. *et al.*: Femtosecond Terahertz Radiation from Femtoslicing at BESSY, Phys. Rev. Lett. 96 (2006), 054801.

[3] Schnegg, A. *et al.*: Frequency domain Fourier transform THz-EPR on single molecule magnets using coherent synchrotron radiation, Phys. Chem. Chem. Phys. 11 (2009), 6820.

[4] Pedersen, K.S. *et al.*: A linear single-molecule magnet based on $[Ru(III)(CN)_6]^{3-}$, Chem. Commun. 47 (2011), 6918.

[5] Dreiser, J. *et al.*: Frequency-Domain Fourier-Transform Terahertz Spectroscopy of the Single-Molecule Magnet $(NEt_4)[Mn_2(5\text{-Brsalen})_2(MeOH)_2Cr(CN)_6]$ Chem. Eur. J. 17 (2011), 7492.

THz Beamline - Reference guide for latest publications

THz Spectroscopy and EPR |
THz Electron Paramagnetic Resonance

The THz beamline exploits intense coherent synchrotron radiation (CSR) as emitted from special storage ring modes, for the study of magneto optical phenomena in the energy range from 3 to 150 cm^{-1}. A dedicated THz electron paramagnetic resonance (THz-EPR) facility combines a broad range of excitation and detection schemes with extreme sample environments (in particular high magnetic fields and low temperatures). Research topics are related to manipulation and detection of high spin states in *e.g.*, proteins, single molecule magnets, energy materials and materials relevant for future information technologies.

The THz beamline extracts CSR from the 2° dipole source (D112) after the slicing section at an acceptance of 60 mrad (h) x 15 mrad (v). A true optical transmission line transports CSR as emitted by ultra-short bunches in the low a mode (pulse length: < 10 ps, spectral range: 3-50 cm^{-1})[1] and laser-induced by femtoslicing [2] (pulse length: ~ 200 fs, spectral range: 20-150 cm^{-1}), respectively. Complementary, FIR-UV-VIS cw radiation and 1 mJ of synchronized fs laser pulses (800 or 400 nm) are available at the experiment. Sample environments include a superconducting magnet (Oxford Spectromag, -11 T to +11 T) equipped with a variable temperature insert (1.5 - 200 K), and an optical cryostat (Oxford Optistat, T = 1.5 - 300 K). THz detection is achieved either with a high resolution FTIR-spectrometer (Bruker IFS 125-HR, min. bandwidth: 0.0063 cm^{-1}) in combination with ultra-sensitive liquid helium cooled Si- or InSb – bolometers or fast Schottky diode THz detectors (ACST, time resolution 250 ps). Alternatively, transient THz signals may be directly detected via a time domain (TD) THz set-up. This dedicated TD THz scheme allows for a cross-correlation of THz pulses from the storage ring with the synchronized external fs-laser source (optical pump – THz probe).

Instrument application

Main science drivers are investigations in spin coupling energies of high spin transition metal and rare earth ions. Spin coupling energies are sensitive probes of the electronic structure and determine magnetic properties of compounds with unpaired electron spins. The latter are highly desired pieces of information, as high spin paramagnetic ions determine the function of many vital catalytic processes in proteins and synthetic complexes, as well as the properties of systems with large exchange couplings, *e.g.* single molecule magnets, energy materials or . The ideal technique to explore magnetic structure-function relationships of materials containing unpaired electron spins is EPR.

However, conventional single frequency EPR frequently fails in cases where spin transition energies exceed the quantum energy of the spectrometer (typically < 4 cm^{-1}). Recently, we have demonstrated that CSR based FD-FT THz-EPR [3] provides a unique tool to overcome this restriction. Our novel approach allows for EPR excitations over a broad energy (3 cm^{-1} – 150 cm^{-1}) and magnetic field range (-11 T - +11 T) in a single spectrometer. FD-FT THz-EPR has been successfully applied to high spin ions in single molecule magnets [4, 5, 6] catalytic mononuclear integer HS TMI complexes and very recently even in proteins and in strongly correlated solid state systems.

Instrument data

Location	12.1
Source	D112
Monochromator	FTIR-Spectrometer IFS125 HR (Bruker Optics) and VERTEX 70
Energy range	5 1/cm 10000 1/cm
Energy resolution	0.0063 1/cm
Flux	5 mW/mm²
Polarization	Variable
Divergence horizontal	60 mrad
Divergence vertical	15 mrad
Focus size (hor. x vert.)	> 0.3 x 0.3 mm
Distance Focus/last valve	900 mm
Height Focus/floor level	1200 mm
Free photon beam available	Yes
Fixed end station	Yes
Instrument responsible	Dr. Karsten Holldack, karsten.holldack@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

THz Spectroscopy & EPR - Reference guide for latest publications

References / Latest publications

[1] Abo-Bakr, M. *et al.*: Brilliant, Coherent Far-Infrared (THz) Synchrotron Radiation, Phys. Rev. Lett. 90 (2003), 094801.

[2] Holldack, K. *et al.*: Femtosecond Terahertz Radiation from Femtoslicing at BESSY, Phys. Rev. Lett. 96 (2006), 054801.

[3] Schnegg, A. *et al.*: Frequency domain Fourier transform THz-EPR on single molecule magnets using coherent synchrotron radiation, Phys. Chem. Chem. Phys. 11 (2009), 6820.

[4] Pedersen, K.S. *et al.*: A linear single-molecule magnet based on $[Ru(III)(CN)_6]^{3-}$, Chem. Commun. 47 (2011), 6918.

[5] Dreiser, J. *et al.*: Frequency-Domain Fourier-Transform Terahertz Spectroscopy of the Single-Molecule Magnet $(NEt_4)[Mn_2(5\text{-Brsalen})_2(MeOH)_2Cr(CN)_6]$ Chem. Eur. J. 17 (2011), 7492.

[6] Dreiser, J. *et al.*: Three-Axis Anisotropic Exchange Coupling in the Single-Molecule Magnets $NEt_4[Mn^{III}_2(5\text{-Brsalen})_2(MeOH)_2M^{III}(CN)_6]$ (M=Ru, Os), Chem. Eur. J. 19 (2013), 3693.

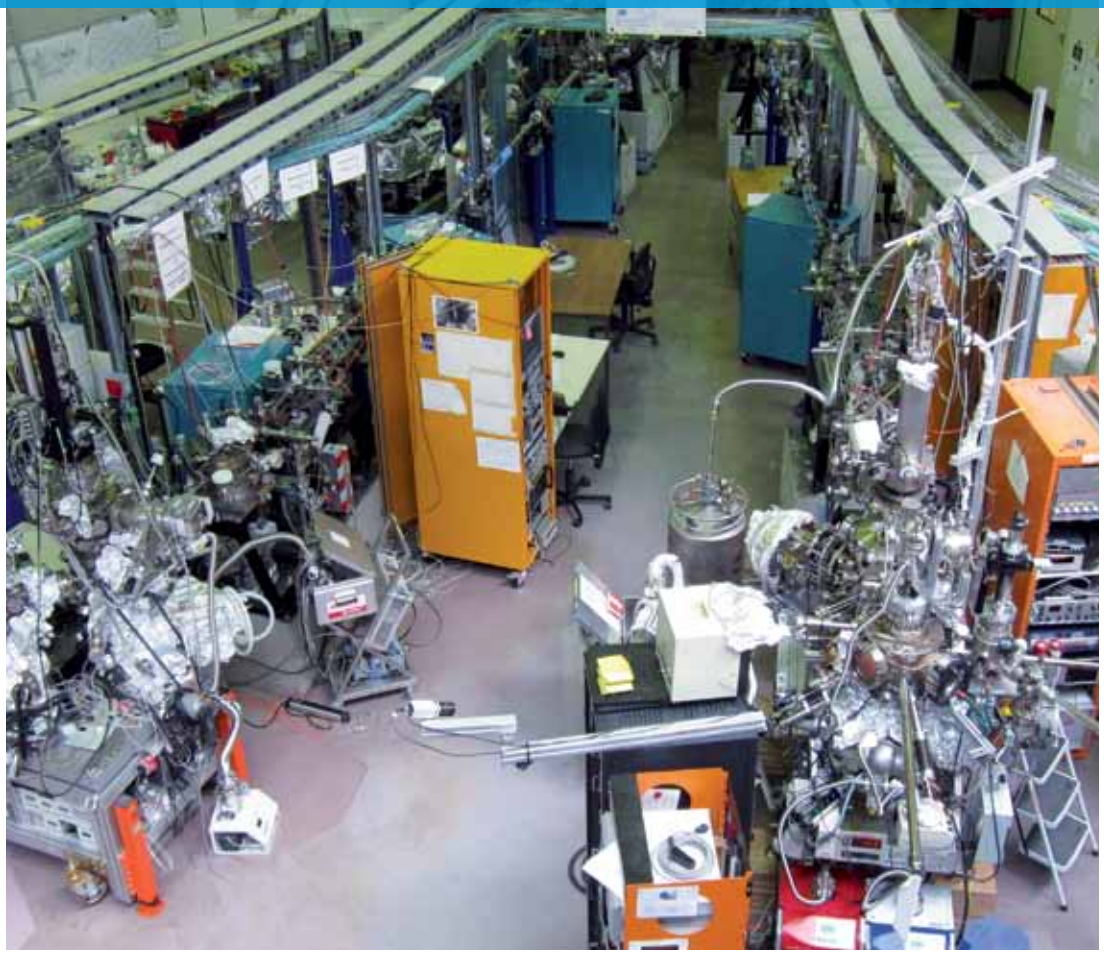
BESSY II

CRG Beamlines Open Port

UE56-2 PGM-1 and **UE56-2 PGM-2 | MPG**

The UE56-2 PGM-1 is a plane mirror/plane grating monochromator. Together with the UE56-2 double undulator it delivers soft X-ray of hight flux, high brilliance, high resolution and different polarisations in a large energy range. From the PGM-1 beamline it differs only in the smaller focus size. It belongs to the Max Planck society (MPG) but is also used by several external and in-house research groups.

The UE56-2 PGM-2 is a plane mirror/plane grating monochromator. Together with the UE56-2 double undulator it delivers soft X-ray of hight flux, high brilliance, high resolution and different polarisations in a large energy range. From the PGM-2 beamline it differs only in the larger focus size. The beamline belongs to the Max Planck society (MPG) but is also used by several external and in-house research groups.



Instrument data

Location	6.2
Source	UE56-2
Monochromator	PGM-1
Energy range	60 - 1300 eV
Energy resolution	80000 at 64 eV
Flux	10^{13} photons
Polarisation	• horizontal • vertical • circular
Divergence horizontal	10 mrad
Divergence vertical	10 mrad
Focus size (hor. x vert.)	PGM-1: 50µm x slit size PGM-2: 900µm x slit size
Distance Focus/last valve	964 mm
Height Focus/floor level	1400 mm
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Willy Mahler, willy.mahler@helmholtz-berlin.de Birgitt Zada, birgitt.zada@helmholtz-berlin.de

Instrument application

- Photoelectron spectroscopy
- Surface Science
- Material Science
- PEEM

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

References / Latest publications

[1] Ostler, M. *et al.*: Buffer layer free graphene on SiC(0001) via interface oxidation in water vapor, Carbon 70 (2014), 258-265.

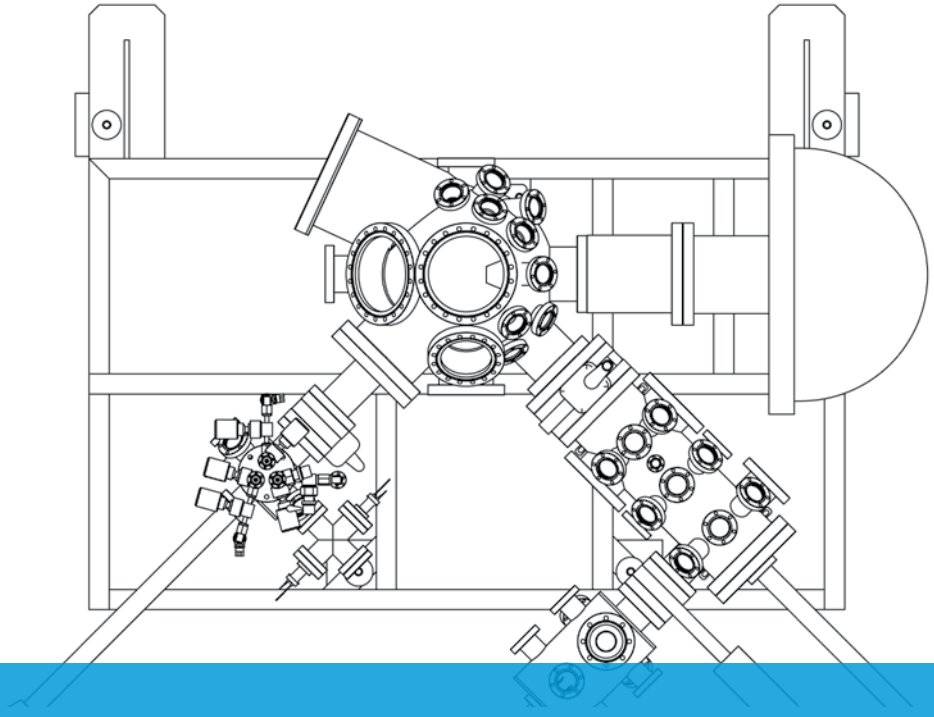
[2] Krüger, A. *et al.*: X-ray-Induced Reversible Switching of an Azobenzene Derivative Adsorbed on Bi(111), J. Phys. Chem. C 118 (2014), 12916-12922.

[3] Huth, M. *et al.*: Electron pair emission detected by time-of-flight spectrometers: Recent progress, Applied Physics Letters 104 (2014), 061602.

[4] Böttcher, S. *et al.*: Reversible photon-induced oxidation of graphene by NO_2 adsorption, Surf. Sci. 621 (2014), 117-122.

[5] Kim, K.S. *et al.*: Visualizing Atomic-Scale Negative Differential Resistance in Bilayer Graphene, Phys. Rev. Lett. 110 (2013), 036804.

UE56-2 PGM-1 and 2
Reference guide for
latest publications



SAMIC-ASAM | BTU

Spectroscopy and Microscopy Integrating Chamber/ Analytical Spectroscopy and Microscopy

The ASAM experimental set up is made by two measurements chambers:
a) a NEXAFS chamber where X-ray Absorption Spectroscopy can be measured with both Fluorescence Yield (FY) and Total Electron Yield (TEY) simultaneously. For FY a channelplate detector is used, while for TEY the drift current is measured.
b) a Photoemission chamber equipped with a PHOYBOS electron analyser (SPECS GmbH). The analyser can use either a channel plate and a CCD detector or a 1D-delay line detector. In this chamber it is possible to measure core level and valence band spectra, resonant photoemission and X-ray spectra using both Partial Electron Yield (PEY) and TEY.
The photoemission chamber is attached to two preparation chambers where cleaning of surfaces and thin film deposition can be done (*e.g.* sputtering, annealing, ALD, CVD, evaporation). The NEXAFS chamber is positioned between the photoemission chamber and the beamline. It is equipped with a separate load lock to introduce the samples. It is not possible to move the samples between the photoemission and the NEXAFS chambers. The NEXAFS chamber can be operated at high pressures (10^{-3} mBar).

Instrument data

Monochromator	PGM 300 l/mm and 1200 l/mm
Experiment in Vacuum	Yes
Temperature range	Room Temperature
Detectors	1-D delay line / CCD camera
Manipulators	3 axis manipulator
Instrument responsible	Dr. Massimo Tallarida, tallamas@tu-cottbus.de

EXPERIMENTAL HALL BESSY II

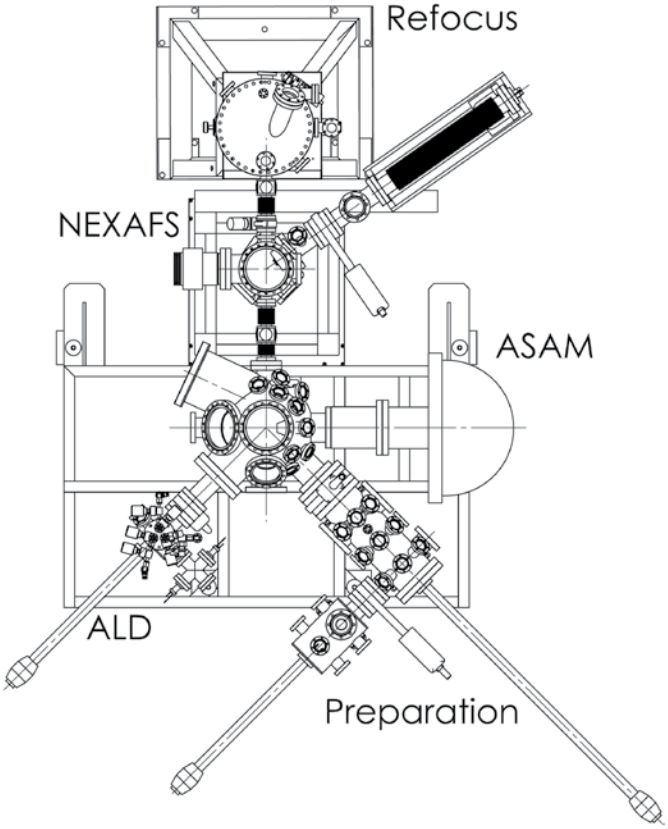
FLEXIBLE STATIONS CRG BESSY II

Instrument application

Methods
- Photoemission Spectroscopy (PES)
- Resonant Photoemission Spectroscopy (ResPES)
- X-ray Absorption Spectroscopy (XAS)

Samples
- Oxides, semiconductors, metals.
- Powders, thin films, single crystal, nanoparticles.

Preparation
- Atomic Layer Deposition (ALD)
- Chemical Vapor Deposition (CVD)
- Evaporation
- Reactive sputtering



References / Latest publications

[1] Tallarida, M. *et al.*: Quantum size effects in TiO_2 thin films grown by atomic layer deposition, D. Beilstein J. Nanotechnol. 5 (2014), 77-82.

[2] Tallarida, M., Schmeisser, D.: *In -situ* ALD experiments with synchrotron radiation photoelectron spectroscopy, Semiconductor Science and Technology 27 (2012), 074010.

[3] Adelmann, C. *et al.*: Surface Chemistry and Interface Formation during the Atomic Layer Deposition of Alumina from Trimethylaluminum and Water on Indium Phosphide, M. Chem. Mater 25 (2013), 1078-1091.

SAMIC-ASAM - Reference guide for latest publications

Synchrotron Facility BESSY II

So-Li-AS | TUD

Solid Liquid Analysis System

The surface science division of the material science faculty of the Technical University of Darmstadt operates a dedicated UHV system for photoemission spectroscopy (PES) experiments with synchrotron radiation as excitation at the Berlin synchrotron facility (BESSY II) located in Berlin-Adlershof. The so called SoLiAS system (solid liquid analysis system) is especially designed for the investigation of the solid-liquid interface and offers the possibility to deposit volatile materials on surfaces of interest and freeze them (LN_2) in order to make PES or low energy electron diffraction (LEED) analysis. Furthermore, an electrochemical treatment of samples under nitrogen atmosphere is possible in a dedicated electrochemistry cell which is attached to the SOLIAS. To keep a high degree of flexibility it is mounted on a moveable frame to make the attachment to various beam lines possible. At BESSY II mainly the U49-2/PGM-2 beam lines with photon energies of 190 - 2000 eV is used for soft X-ray photoemission spectroscopy (SXPS) experiments with varying excitation energy. In addition to the mentioned PES experiments also X-ray absorption (XAS) experiments can be carried out. At the moment the SoLiAS system is mainly used for fundamental research on Li-batteries, organic solar cells, semiconductors for water splitting and absorber materials for thin film photovoltaics.

Instrument data

Monochromator	Depending on beamline: U49-2 PGM-2 (Undulator beamline)
Experiment in vacuum	Yes
Temperature range	77 – 700 K
Detector	SPECS Phoibos 150 with DLD Detector (energy range 15-3000 eV) SPECS ErLEED (three grids)
Manipulators	Manufacturer: VAb Δz=600 mm (motorized) Δx=50 mm, Δy=50 mm (manually) rotation ΔΦ=360° (manually) azimuth Δϑ=180° (manually)
Heating and sputter station	RT – 1000 K SPECS Ar-sputter gun
Electrochemistry cell	Ar or N purged glass vessel attached to the SoLiAS for *in-situ* investigations
Instrument responsible	Dr. Thomas Mayer, mayerth@surface.tu-darmstadt.de Dr. Christian Pettenkofer, pettenkofer@helmholtz-berlin.de

Instrument application

- Investigation of solids (amorphous, crystalline), especially semiconductor and metals
- Studying of interface and surface reactions after wet-chemical treatment (*e.g.* chemical shift)
- Varying of the information depth by tuning the excitation energy
- Measurement of the electronic properties of the surface (*e.g.* band line-up, valence band maximum, or work function)
- X-ray absorption measurements (total electron yield)
- Attachment of customer UHV systems for special scientific tasks (deposition or adsorption of new materials)
- Electrochemistry in combination with PES and LEED with an *in-situ* approach

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS CRG BESSY II

References / Latest publications

[1] Gajda-Schrantz, K. *et al.*: Formation of an electron hole doped film in the a-Fe_2O_3 photoanode upon electrochemical oxidation, Phys. Chem. Chem. Phys., 15 (2013), 1443-1451.

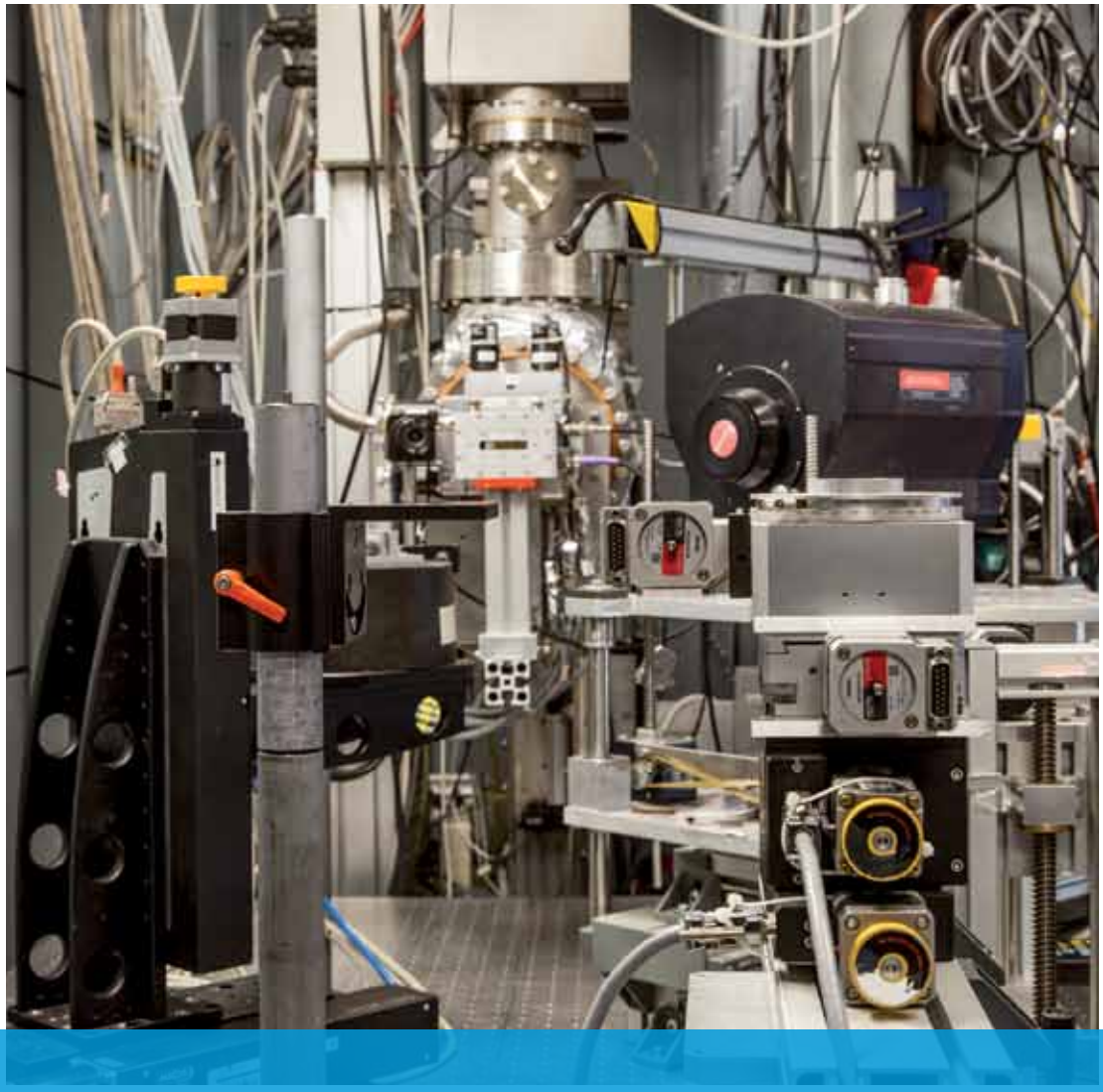
[2] Lebedev, M.V. *et al.*: Sulfur Passivation of GaSb(100) Surfaces: Comparison of Aqueous and Alcoholic Sulfide Solutions Using Synchrotron Radiation Photoemission Spectroscopy, J. Phys. Chem. C, 117 (2013), 15996-16004.

[3] Kaiser, B. *et al.*: Solar Hydrogen Generation with Wide-Band-Gap Semiconductors: GaP(100) Photoelectrodes and Surface Modification, Chemphyschem, 13 (2012), 3053-3060.

So-Li-AS - Reference guide for latest publications

BESSY II

CRG Beamlines Fixed Stations



BAMline | BAM

Nondestructive testing in analytical chemistry

The BAMline is a multipurpose hard X-ray beam line dedicated to nondestructive materials characterization. The X-ray source of the beam line is a superconducting 7T wavelength shifter (WLS), hence the photon energy ranges from 5 keV up to 80 keV. The main optical components are a double multilayer monochromator (DMM, $\Delta E/E$ = 60 keV) and a double crystal monochromator (DCM, $\Delta E/E = 5 \cdot 10^{3}$ eV). Both monochromators can be operated independently or in series. The X-ray beam can be focused to a spot size of about 200 µm (by bending the monochromator mirror/crystal). The BAMline is specialized for nondestructive material characterization using different methods.

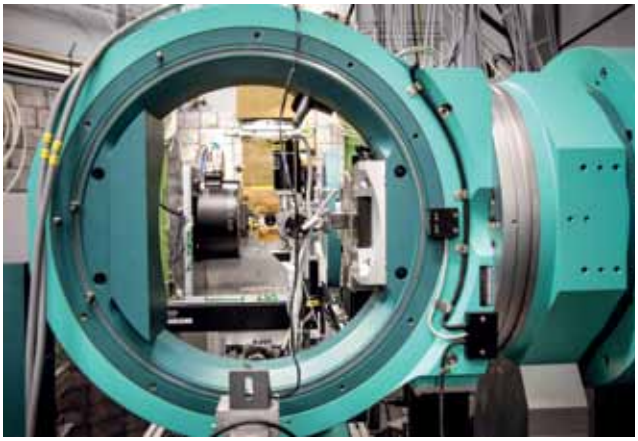
Instrument data

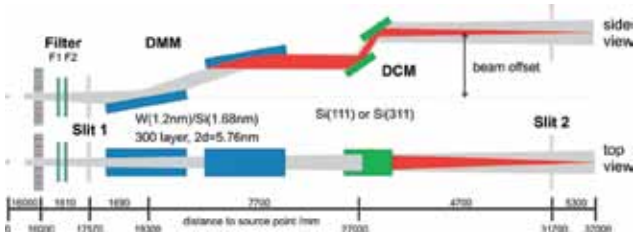
Monochromator	Double Crystal Monochromator Si 111 and Double Multilayer Monochromator
Source	7T-WLS-1
Location	3.2
Flux	10^{12}
Polarization	Horizontal
Experiment in vacuum	No
Temperature range	Ambient
Detector	Color X-ray Camera pnCCD, e2V Si-Li, Bruker X-Flash, CCD, optical microscope
Energy range	5-100 keV
Instrument responsible	Dr. Heinrich Riesemeier, heinrich.riesemeier@helmholtz-berlin.de Dr. Bernd Müller, bernd.mueller@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

FIXED STATIONS CRG BESSY II





Instrument application

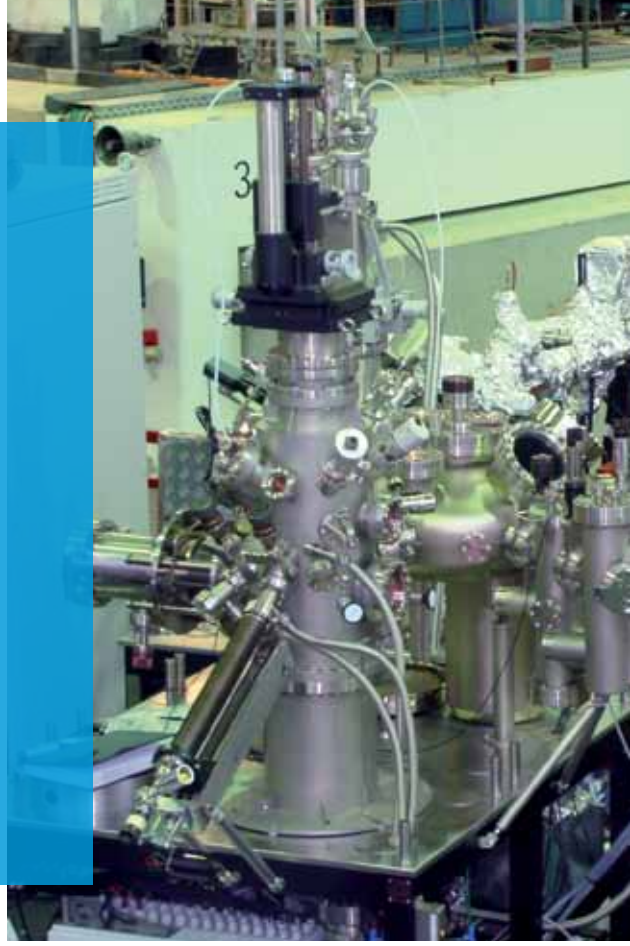
For materials characterization several experimental setups are available: X-ray Micro Tomography, with special resolution from 7 µm down to 0.3 µm; X-ray Refraction Topography; X-ray Diffraction, Small Angle X-ray Scattering, X-ray Reflectometry, X-ray Fluorescence Analysis, extended X-ray absorption fine structure.

BAMline - Reference guide for latest publications

HE-SGM | KIT

The HE-SGM beamline is a dipole beamline optimized for NEXAFS spectroscopy in the VUV range. It was designed to cover the light element (C, N, O and F) K-edges which contains important spectroscopic information about soft matter samples, carbon (nano) materials and molecules adsorbed on catalytically relevant surfaces. The beamline monochromator allows for fast scanning over the energy ranges of interest (100-800 eV). There are a number of similar beamlines at other synchrotron radiation facilities worldwide. With regard to the spectroscopic parameters the HE-SGM beamline is considered to be in the top third of comparable dipole beamlines.

The optical elements of the beamline (mirror, monochromator) were additionally cleaned with oxygen plasma to remove carbon contamination from their surface resulting in a crucial decrease of parasitic contribution to the experimental data. Such uniqueness allows to acquire proper experimental data for organic molecular thin films with a thickness down to 0.1 monolayer. During reinstallation of the beamline the adjustment of the entrance slit was improved resulting in a better polarization factor – which increased to 91%.



Instrument application

- NEXAFS and soft-XPS investigations of organic molecules on metal and metal oxides, metal-organic complexes, polymers and carbon-based 2D materials.

References / Latest publications

[1] Nefedov A., Wöll C.: Advanced Applications of NEXAFS Spectroscopy for Functionalized Surfaces, in Surface Science Techniques, (Eds) G. Bracco and B. Holst Springer Series in Surface Science, v. 51, Springer-Verlag, Berlin, Heidelberg, New York, Tokyo, (2013), pp. 277.

[2] Klappenberger F.: Two-dimensional functional molecular nanoarchitectures - complementary investigations with scanning tunneling microscopy and X-ray spectroscopy, Prog. Surf. Sci. 89 (2014), 1-55.

HZB Helmholtz Zentrum Berlin

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

HE-SGM - Reference guide for latest publications

Instrument data

Location	4.1
Source	D2.1
Monochromator	HE-SGM
Energy range	100 - 750 eV
Energy resolution	500 - 2500
Flux	$5x10^{11}$ photos/(s • 100 mA)
Polarization	Horizontal
Stray light	None due to baffles
Stability	Thermal stability after 30 min.
Higher orders	2^{nd} order 2%, 3^{rd} order 0.02%
Divergence horizontal	1.5 mrad
Divergence vertical	1.5 mrad
Focus size (hor. x vert.)	1.2 × 0.5 mm
Distance Focus/last valve	500 mm
Height Focus/floor level	1400 mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Alexei Nefedov, alexei.nefedov@kit.edu

HE-SGM Station | KIT

NEXAFS / XPS experimental station

The NEXAFS/XPS experimental station is a multi-chamber UHV system produced by PREVAC (Poland) and consists of the following chambers:

1. Two loadlocks: the first one is used for fast sample exchange with a storage facility for up to six sample holders, the second one is used for sample exchange with a storage facility for 2 sample holders and with an opportunity to install a special vacuum transfer box allowing to transport samples under UHV conditions. Moreover, the park station connected to the distribution chamber allows the storage of additional 6 sample holders under UHV conditions.

2. The unique sample transfer system including the distribution chamber of the carousel type (a base pressure of better than 10^{-10} mbar) and manipulators allow fast (less than 1 minute) transfer of samples from one chamber to another one. It was established that during the sample transfer in the cold (~ 100 K) state the temperature doesn‘t increase by more than 20 K.

3. A versatile preparation chamber operated at a base pressure of better than 5 x 10^{-9} mbar accepting up to 5 evaporators for metals or-organics and/or other sources (for example, atomic H source etc.), two sputter guns, gas dosing systems as well as a LEED system for control of the sample quality. One of the evaporators is permanently installed and available to all HE-SGM users. A special receiving station of the manipulator allows for cooling with liquid nitrogen to 100 K and for heating up to 2000 K.

4. A main chamber with a base pressure of better than 10^{-10} mbar is equipped with a hemispheric electron energy analyser (Scienta R3000, a sputter gun, and a home built double channel plate detector enabling NEXAFS spectroscopy in partial electron yield (PEY) or total electron yield (TEY) mode. The energy analyser and the MCP-NEXAFS detector can be read out at the same time thus allowing a simultaneous recording of integrated secondary electrons (PEY or TEY) and energy resolved Auger electrons. For the measurements the sample is transferred to a 5-axes manipulator with three translational and two rotational (polar and azimuthal angles) degrees of freedom. A continuous-flow liquid He cryostat installed in the chamber allows sample cooling down to 30 K, while depending on the sample holder samples can be heated up to 2000 K.

Instrument application

- Metal-organic frameworks and their loading with gases and metal nanoparticles
- Adsorption of organic molecules and metal oxides
- Novel carbon-based materials (including their functionalization)
- Development of NEXFAS investigation of ionic liquids
- Charge transfer dynamics in molecular films
- Dipole control at surfaces and interfaces using monomolecular films
- Optically controlled molecular switches
- Ultrathin molecular and polymeric membranes
- Novel molecular functional films
- Lithography with a monomolecular resist
- Metallo-organic oligomer films: design and applications

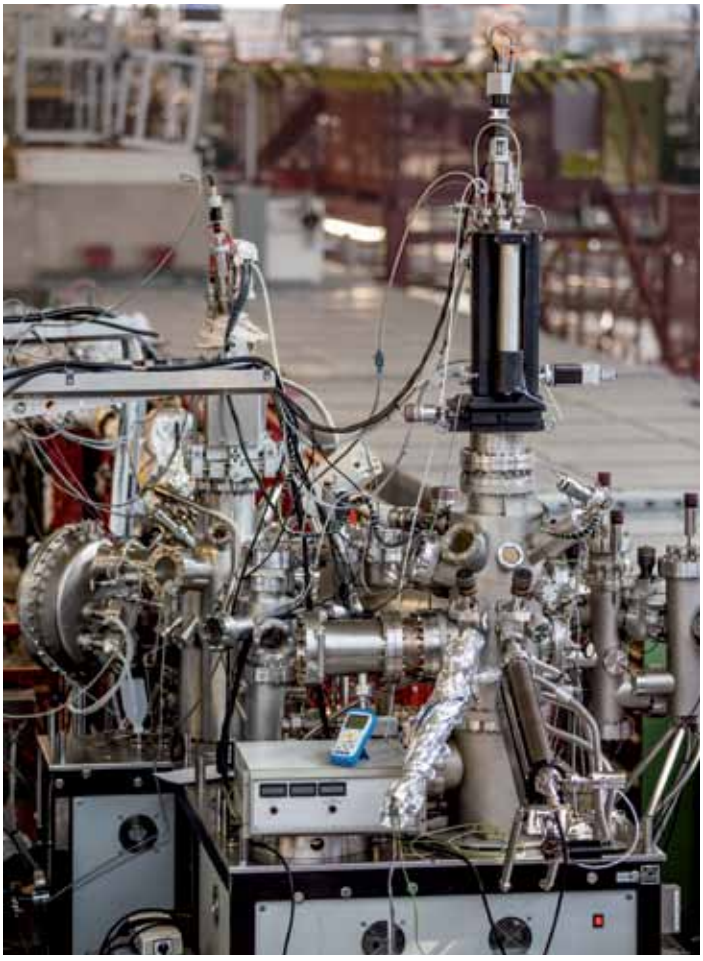
Instrument data

Monochromator	SGM
Experiment in vacuum	Yes
Temperature range	50 – 1200 K (for T>1200 K contact Station Manager)
Detector	XPS: Scienta R3000, NEXAFS: channel-plate-based electron detector (for use a fluorescence detector contact Station manager)
Scattering Geometry	Horizontal
Angular range	-45° - 135° in respect to direct beam direction
Standard sample size	10mm x 10mm (in a case of other sizes contact Station Manager)
Azimuthal sample rotation	Yes
Software	SES for XPS, LabView-based and EMP2 for NEXAFS
Instrument responsible	Dr. Alexei Nefedov, alexei.nefedov@kit.edu

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

FIXED STATIONS CRG BESSY II



References / Latest publications

[2] Klappenberger, F.: Two-dimensional functional molecular nanoarchitectures - complementary investigations with scanning tunneling microscopy and X-ray spectroscopy, Prog. Surf. Sci., 89 (2014), 1-55.

[1] Nefedov, A., Wöll, C.: Advanced Applications of NEXAFS Spectroscopy for Functionalized Surfaces, in Surface Science Techniques, (Eds) G. Bracco and B. Holst Springer Series in Surface Science, v. 51, (Springer-Verlag, Berlin, Heidelberg, New York, Tokyo), (2013), pp. 277.

HE-SGM Station - Reference guide for latest publications

ISISS | MPG

ISISS (Innovative Station for *In-Situ* Spectroscopy) is a project of the Inorganic Chemistry department of the FHI (Fritz-Haber-Institut der Max-Planck-Gesellschaft) and HZB/BESSY II in Berlin. The purpose of the ISISS facility is to provide access for a large community to surface sensitive gas/solid interface characterisation methodologies in the presence of a reactive gas, i.e. *in-situ* under conditions equal to or close to reality. The working area of the facility is material science in general and catalysis in particular.

Our approach includes 3 units that have to complement one another: a state of the art soft X-ray beamline, an endstation for ambient pressure X-ray photoelectron (NAP-XPS) and X-ray absorption spectroscopy (XAS), and an infrastructure on site to perform experiments with a chemical background. In contrast to standard vacuum surface science experiments, *in-situ* experiments require the installation of a complex gas feed and an elaborated gas analytic to follow the conversion of the gas phase during the reaction.

Instrument application

- Dynamic response of surfaces on chemical potential of environment
- *In-situ* surface characterisation of gas/solid interfaces in heterogeneous catalysis
- *In-situ* surface characterisation of liquid/solid interfaces (*e.g.* water splitting)
- Electronic structure - performance correlations of functional materials
- Electrochemistry, fuel cells and battery research

References / Latest publications

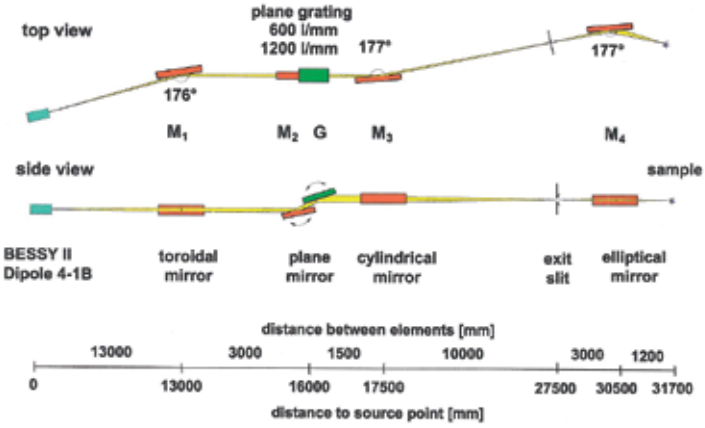
[1] Zander, S. *et al.*: The role of the oxide component in the development of copper composite catalysts for methanol synthesis, Angewandte Chemie (International ed. In English) 52 (2013), 6536-6540.

[2] Yashina, L.V. *et al.*: Negligible Surface Reactivity of Topological Insulators Bi_2Se_3 and Bi_2Te_3 towards Oxygen and Water. ACS nano 7 (2013), 5181-5191.

[3] Starr, D.E. *et al.*: Investigation of solid/vapor interfaces using ambient pressure X-ray photoelectron spectroscopy, Chemical Society reviews 42 (2013), 5833-5857.

Instrument data

Location	6.1
Source	D41
Monochromator	PGM
Energy range	80 - 2000 eV
Energy resolution	>15000 at 400 eV
Flux	6x1e^{10} photons/s/0.1A with 111 µm exit slit
Polarisation	Linear horizontal
Divergence horizontal	2 mrad
Divergence vertical	2.4 mrad
Focus size (hor. x vert.)	100x80 µm^2
Distance Focus/last valve	870 mm
Height Focus/floor level	1405 mm
Free photon beam available	No
Fixed end station	No
Instrument responsible	Dr. Michael Hävecker, michael.haevecker@helmholtz-berlin.de



Optical layout

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

ISISS - Reference guide for latest publications

ISISS station | MPG

Innovative Station for In Situ Spectroscopy

Obviously, the understanding of the interaction of a catalyst surface with the reactants plays a key role in a detailed description of catalytic processes. X-ray photoelectron spectroscopy (XPS) is a well-established powerful tool to study in detail the outermost surface of solids but it was traditionally restricted to high vacuum and low pressure conditions. However, recently a methodology based on a differentially pumped electrostatic lens system has gained much interest.

The Fritz-Haber-Institut (MPG) has operated at BESSY such an instrument since 2002 at different undulator based beamlines. In 2007 a beamline (ISISS) dedicated to near ambient pressure XPS (NAP-XPS) and X-Ray absorption spectroscopy (XAS) experiments has been implemented at BESSY II. A further improved version of this instrument is installed as the ISISS beamline since June 2013.

Instrument data

Monochromator	ISISS plane grating monochromator
Experiment in vacuum	Yes
Temperature range	Up to 1300K, depending on sample
Detector	2D delay line detector (2D DLD)
Manipulators	Various, optimised for sample environment
Maximum pressure	2000 Pa
Minimum pressure	10^{-10} Pa
Typical pressure	100 Pa
Gas analytics	• Electron impact mass spectrometer (differentially pumped) • Proton-transfer-reaction mass spectrometer (PTR-MS) • Micro gas chromatograph
Instrument responsible	Dr. Michael Hävecker, michael.haevecker@helmholtz-berlin.de

ISISS station - Reference guide for latest publications

EXPERIMENTAL HALL BESSY II

FIXED STATIONS CRG BESSY II

Instrument application

- Dynamic response of surfaces on chemical potential of environment
- *In-situ* surface characterisation of gas/solid interfaces in heterogeneous catalysis
- *In-situ* surface characterisation of liquid/solid interfaces (*e.g.* water splitting)
- Electronic structure - performance correlations of functional materials
- Electrochemistry, fuel cells and battery research

References / Latest publications

[1] Armbruester, M., *et al.*: $Al_{13}Fe_4$ as a low-cost alternative for palladium in heterogeneous hydrogenation, Nature Materials 11 (2012) 690-693.

[2] Barbosa, R.L., *et al.*: Methanol Steam Reforming over Indium-Promoted Pt/Al_2O_3 Catalyst: Nature of the Active Surface. Journal of Physical Chemistry C 117 (2013), 6143-6150.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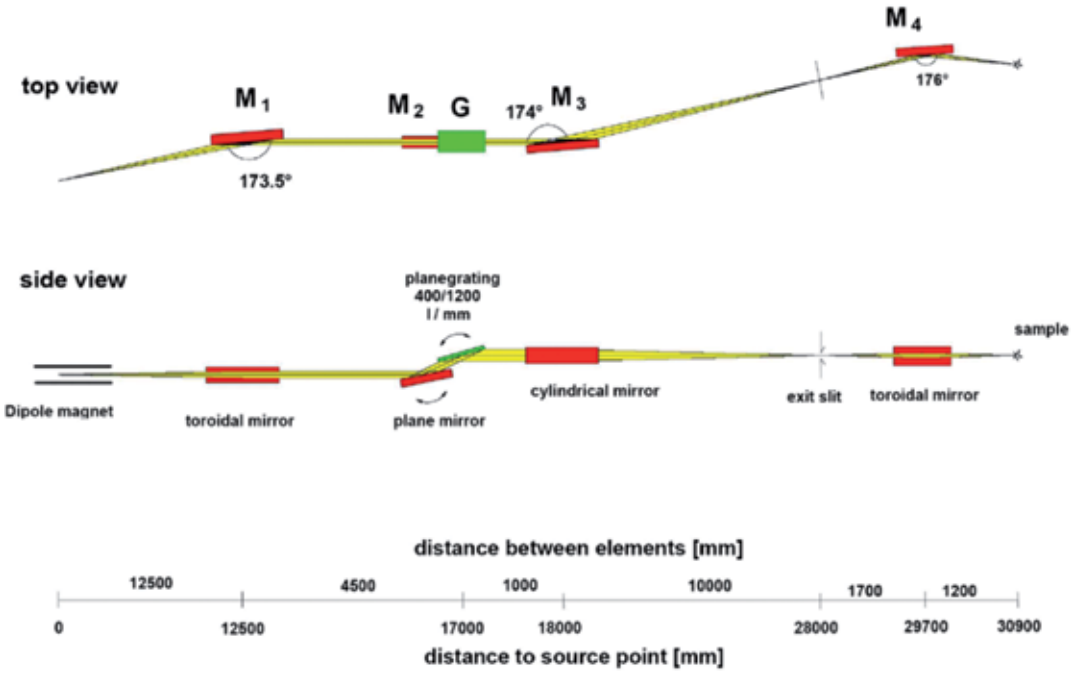
Synchrotron Facility BESSY II



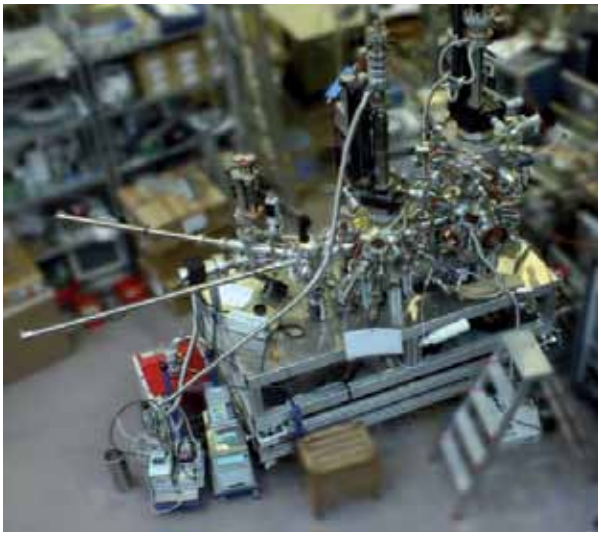
RGL | Russian-German Dipole Beamline

The Russian–German Soft X-ray Beamline (RGBL) was assembled at a bending magnet of the storage ring BESSY II and was constructed in a close cooperation between scientists from Freie Universität Berlin, St. Petersburg State University, BESSY GmbH, and Technische Universität Dresden. The optical design of the RGBL is based on the Petersen-type plane-grating monochromator (PGM). The toroidal mirror M1 upstream of the monochromator provides a 3 mrad horizontal acceptance of the source. This mirror focuses the source horizontally onto the exit slit, while the sagittal radius collimates the beam vertically. The collimated light from M1 is diffracted by the vertically deflecting gratings (400 and 1200 grs/mm) in the Petersen-type PGM geometry [plane mirror (M2)–plane grating]. The cylindrical mirror M3 focuses the diffracted light vertically onto the exit slit. The image at the exit slit is refocused by the toroidal mirror M4 onto the sample position in the experimental station.

The Russian–German Beamline has an extraordinary high spectral-resolution and photon-flux performance. In particular, a resolving power up to 100000 (at hν = 64 eV) has been demonstrated using the extremely narrow double-excitation resonances of He. It is worth noting that in contrast to undulator beamlines mostly employed nowadays, this dipole beamline provides radiation of moderate intensity continuously distributed over a wide range of photon energies from 30 to 1500 eV. It is therefore well suited for studies of “fragile” biological objects, which usually show high sensitivity to X-ray damage.

Instrument data

Location	1.2
Source	D161
Monochromator	PGM
Polarisation	Horizontal
Distance Focus/last valve	820 mm
Height Focus/floor level	1400 mm
Data acquisition software	EMP / 2
Free photon beam available	Yes
Fixed end station	No
Instrument responsible	Dr. Denis Vyalikh, denis.vyalikh@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

References / Latest publications

[1] Gorovikov, S.A. *et al.*: Optical design of high-energy resolution beamline at a dipole magnet of BESSY II, Nucl. Instr. and Meth. A 411 (1998), 506-512.

[2] Gorovikov, S.A. *et al.*: Optimization of the optical design of the Russian-German soft-X-ray beamline at BESSY II, Nucl. Instr. and Meth. A 467-468 (2001), 565-568.

[3] Fedoseenko, S.I. *et al.*: Development and present status of the Russian-German soft X-ray beamline at BESSY II, Nucl. Instr. and Meth. A 470 (2001), 84-88.

[4] Vyalikh, D.V. *et al.*: Commissioning of the Russian-German XUV Beamline at BESSY II, Synchrotron Radiation News, 15 (2002), 26-28.

[5] Fedoseenko, S.I. *et al.*: High-energy resolution Russian-German dipole beamline at BESSY in operation, Nucl. Instr. and Meth., 505 (2003), 718-728.

RGL - Reference guide for latest publications

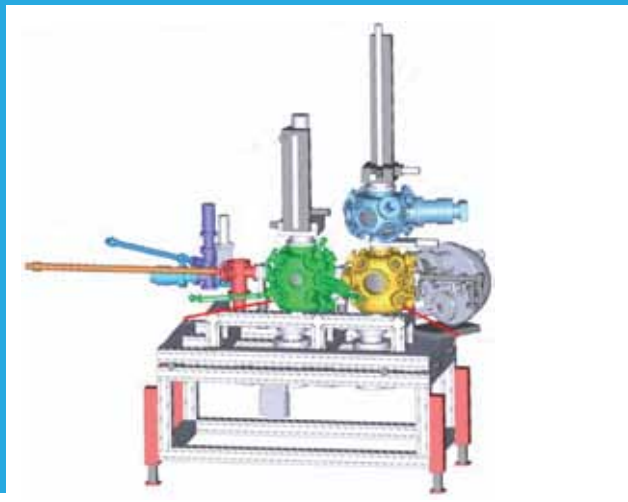
RGL PES | Russian German Photoemission Station

The RGBL station is very flexible and demonstrates reliable performance for the whole variety of experiments of RGBL user community. Having several preparation chambers, fast-load systems, a number of insertion devises such as a flash-machine, a cleavage system, a heating stage, a gas-inlet system etc., the station is a powerful instrument allowing to study fundamental properties of matter. Furthermore, an analytical chamber has been configured in a way that it now allows to study a particular physical processes or chemical reactions in real-time.

The experimental station is equipped with PHOIBOS 150 electron-energy analyzer with the 2D CCD detector system (SPECS GmbH), which simultaneously offers both energy and angular resolution and allows band mapping as well as high resolution XPS/UPS. The MCP-LEED system (Omicron GmbH) allows to explore LEED from rather delicate systems like organic molecules and electrically insulating surfaces. The specific advantage of the multichannel plate (MCP) detector is that it allows electron beam currents down to 0.1 nA. The endstation includes a new cryo-manipulator (lowest temperature about 20 K) which permits polar and azimuthal rotations of the sample and motions along the x, y, and z axes.

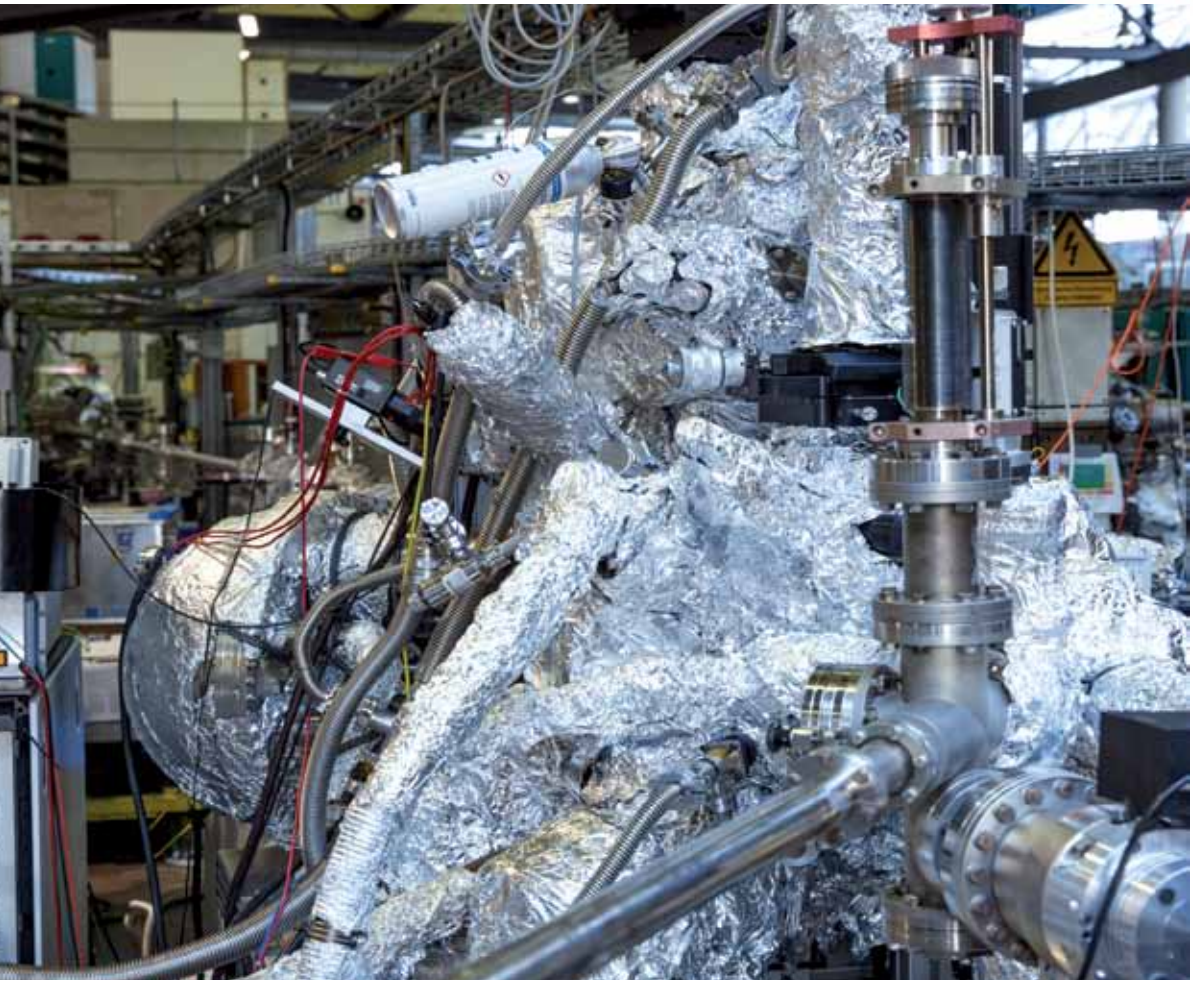
Conceptually, the instrument consists of three main chambers. The “top” preparation chamber is positioned right above the analytical chamber and dedicated for “clean” experiments with rather delicate and reactive materials like rare-earth elements. It is equipped with a quartz microbalance, flanges to mount evaporators, a gas inlet system, a flash-machine, a wobble stick, an ion gun, a few windows, a manipulator and a fast-entry system. Here, thin films can be deposited *in-situ* from Knudsen cell-type evaporators. Surfaces of bulk samples can be prepared by several methods: (a) cleaving; (b) sputtering; (c) heating up to 2000°C; (d) scraping.

Measurements are done in the analytical chamber which is equipped with (i) a PHOIBOS 150 electron-energy analyzer, (ii) an MCP-LEED system, (iii) a partial yield electron detector and (iv) a X-ray tube. A port for the installation of a fluorescence detector is foreseen. This allows time-dependent experiments where metal deposition and PE data acquisition are done simultaneously. A second flexible station (RGBL-2) is still under construction.



Instrument data

Instrument responsible	Dr. Denis Vyalikh, denis.vyalikh@helmholtz-berlin.de



EXPERIMENTAL HALL BESSY II

FIXED STATIONS CRG BESSY II

References / Latest publications

[1] Fedorov, A.V. *et al.*: Observation of a universal donor-dependent vibrational mode in graphene, Nature Communications 5 (2014), 3257.

[2] Bondarenko, L.V. *et al.*: Effect of Na adsorption on the structural and electronic properties of Si(111) $\sqrt{3}\times\sqrt{3}$-Au surface, J. Phys. Condens. Matter 26 (2014), 055009.

[3] Yashina, L.V. *et al.*: Negligible Surface Reactivity of Topological Insulators Bi_2Se_3 and Bi_2Te_3 towards Oxygen and Water, ASC Nano 7 (2013), 5181.

[4] Makarova, A.A. *et al.*: Self-Assembled Supramolecular Complexes with “Rods-in-Belt” Architecture in the Light of Soft X-rays, J. Phys. Chem. C 117 (2013), 12385.

RGL PES-
Reference guide for
latest publications

Molecular beam epitaxy system (MBE)

U125-2 KMC | PDI

The X-ray source is an undulator installed in a high beta section of the orbit of the storage ring BESSY II. This undulator has 32 periods, each with a length of 125 mm, and a variable magnet gap from 100 to 15.7 mm. The critical photon energy of the undulator on the axis is 2.6 keV. The average power emitted by the undulator into an angular range of 1 mrad horizontally and integrated vertically is 160 W at 100 mA beam current. The designed energy range of the beamline is 6–12 keV. The X-ray beam is shaped by means of four independent water-cooled slits located 22 m from the source. A toroidal pre-mirror collimates the beam for either a flat double Si(111) crystal monochromator (DCM) or a multilayer (DMM) optic, which may enhance the photon flux at the sample by about two orders of magnitude compared to the DCM. Behind the monochromator optics there is another chamber which contains two mirrors that can be used alternatively either for focussing or parallelizing the beam at the sample. The experimentally observed focus size is well within 1 mm^2. The center of the diffractometer is placed onto the beam axis by means of two perpendicular motorized linear translations. The sphere of confusion of the

incidence diffraction in the z-axis geometry in an extended range along the crystal truncation rods. The incidence angle α is varied by rotating the entire diffractometer around its vertical axis.

The PHARAO experiment is designed to investigate epitaxial layers during molecular beam epitaxy (MBE). Performed *in-situ*, under real growth conditions, and in real time, the research improves the understanding of fundamental growth processes during MBE. Our work focuses on the study of epitaxial growth modes, structural analysis of interfaces and layer stacks, phase transitions, and phenomena associated with the combination of very dissimilar materials.

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

FIXED STATIONS CRG BESSY II

Instrument application

- Surface X-ray scattering and reflectivity for *in-situ* observation of epitaxial growth processes
- Combination of solid-source molecular beam epitaxy system and six-circle diffractometer

Instrument data

Location	5.1
Source	U125-2
Monochromator	KMC
Energy range	6 - 12 keV
Energy resolution	1500
Polarization	Horizontal
Divergence horizontal	0.8 mrad
Divergence vertical	0.08 mrad
Focus size (hor. x vert.)	0.5 x 0.5 mm^2
Height Focus/floor level	1500 mm
Free photon beam available	No
Fixed end station	No
Instrument responsible	Dr. Michael Hanke, michael.hanke@helmholtz-berlin.de

References / Latest publications

[1] Jenichen, B. *et al.*: Combined molecular beam epitaxy and diffractometer system for in situ studies of crystal growth, Review of Scientific Instruments 74 (2003), 1267-1273.

[2] Proessdorf, A. *et al.*: Epitaxial polymorphism of La2O3 on Si(111) studied by in situ X-ray diffraction, Appl. Phys. Lett. 105 (2014), 021601.

U125-2 KMC - Reference guide for latest publications

MAXYMUS | MPG
Magnetic X-ray Micro- and UHV Spectroscope

MAXYMUS is a scanning transmission X-ray microscope (STXM) operated by the Max-Planck-Institute for Intelligent Systems. It allows high resolution imaging down to below 20 nm spatial resolution by scanning a small X-ray spot, created by a Fresnel zone plate, across a sample and measuring the transmitted signal to determine the X-ray absorption. It is possible to use absorption methods like XMCD and NEXAFS to directly picture magnetic domains, elemental distribution or the local chemical environment of a sample on this lengths scale by choice of X-ray energy and polarization (which the UE46 beamline can provide with high intensity between 150 and 1900 eV both in linear and circular polarization.) In addition to classical transmission operation, which requires samples with <1 µm thickness, MAXYMUS also allows surface sensitive imaging of non-transparent samples by measuring sample current, which is facilitated by full UHV capability to prevent sample contamination.

A particular strength of the instrument is time resolved magnetic microscopy by using the stroboscopic nature of the synchrotron light. A full pump-and-probe setup is provided for users to efficiently image dynamic processes with time resolutions of <100 ps. Sequences of 1000 of frames can be acquired concurrently, with no loss of spatial resolution. Tools for magnetic microscopy like a magnet system providing up to 250 mT of field in arbitrary directions and a goniometric sample holder are also available.

Instrument application

Main application of MAXYMUS is magnetic microscopy. XMCD allows the study of the magnetization direction locally inside a sample, without having to rely on stray field, while also being undisturbed by external fields. Due to the strengths of the XMCD effect and its spatial resolution, MAXYMUS can quickly and with high quality image domain walls, vortex cores and other magnetic features. With its custom pump-and-probe system and its <100 ps time resolution, dynamic processes like domain wall movements, spinwaves or vortex core gyration can be directly observed.

Second application for MAXYMUS is the use of NEXAFS for environmental and material science. Its penetration depth of several 100 nm allows to investigate the elemental distribution in heterogeneous particles of several 100 nm diameter or to image deeper layers of multilayer structures for example.

Instrument data

Monochromator	• Eff. Energy from 150 eV upto 1900 eV • One high flux, 600 l/mm blazed (0.7° angle) and a high resolution 1200 l/mm grating • Variation of the deflection angle by plane mirror
Energy range	150 - 1900 eV
Experiment in vacuum	Yes
Focus size (hor. x vert.)	• At exit slit: ~ H 45 µm x V 15 µm • At zoneplate: ~ H 2 mm x V 1 mm
Temperature range	• Typically room temperature • 80K to RT using cryostat sample holder
Detector	• Photomultiplier E <600 eV • Avalanche Photodiode (APD) for fast (<2 ns) single photon detection and high count rates (> 108 photons/s) • Sample Current (TEY) for non-transparent samples • Fast in Vacuum X-ray CCD upcomming
Time resolution	• Multi Bunch: 35 psec • Low Alpha: 10 psec
Atmosphere	• Ultra High Vacuum (< 10^{-8} mbar) • Helium for sample cooling
Sample handling	UHV sample preparation chamber (sample magazine, Ar-sputtergun, ebeam baking, airfree transfer)
Instrument responsible	Markus Weigand, markus.weigand@helmholtz-berlin.de

The insides of the MAXYMUS vacuum chamber, including piezo stages for sample scanning and interferometer lasers for position control.

EXPERIMENTAL HALL BESSY II

FIXED STATIONS CRG BESSY II

References / Latest publications

[1] Follath, R. *et al.*: The X-ray microscopy beamline UE46-PGM2 at BESSY, AIP Conf. Proc. 1234 (2010), 323.

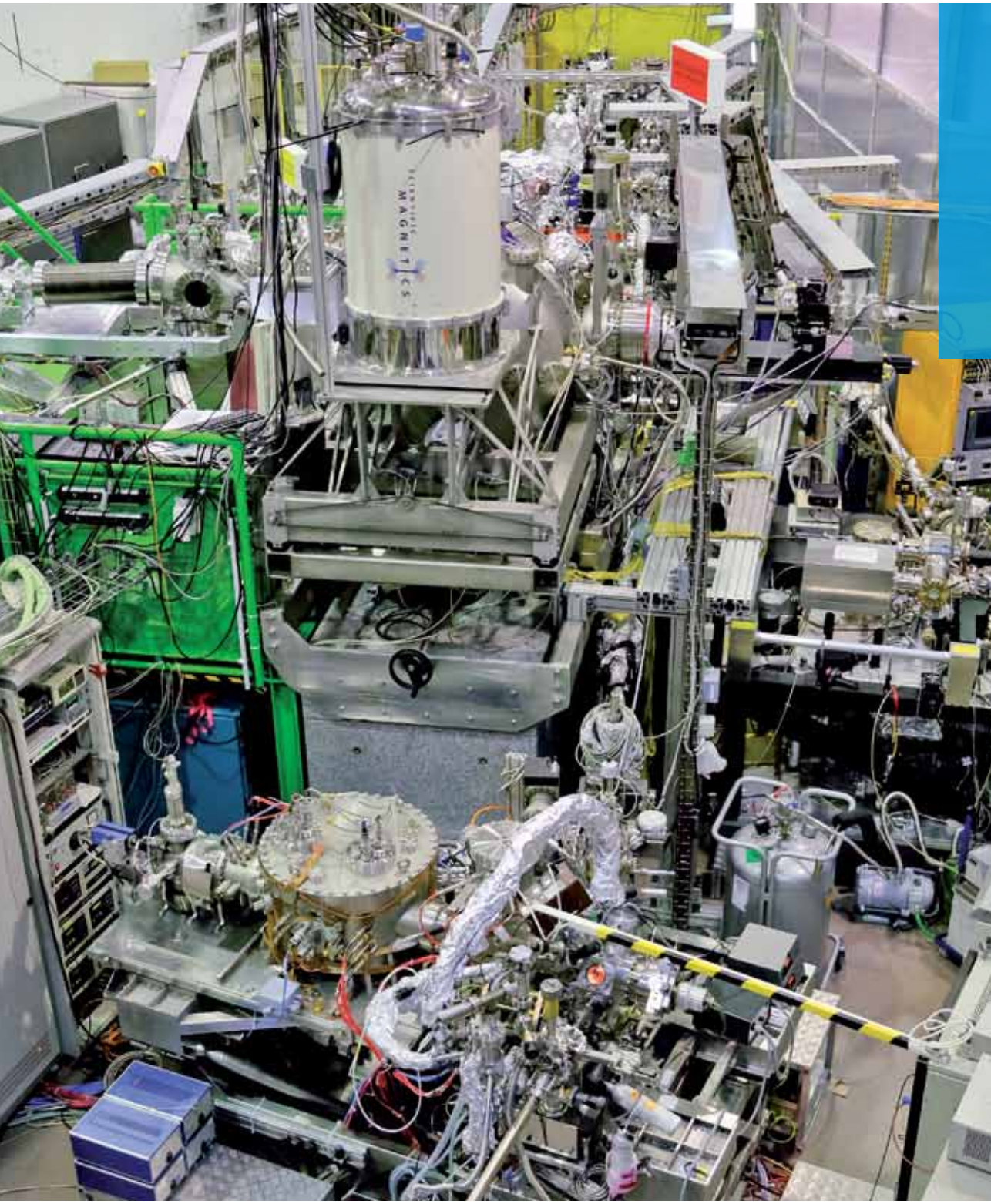
[2] Nolle, D. *et al.*: High Contrast Magnetic and Nonmagnetic Sample Current Microscopy for Bulk and Transparent Samples Using Soft X-rays, Microscopy and Microanalysis 17 (2011), 834-842.

[3] Kammerer, M. *et al.*: Magnetic vortex core reversal by excitation of spin waves, Nature Communications 2 (2011), 279.

[4] Pöhlker, C. *et al.*: Biogenic Potassium Salt Particles as Seeds for Secondary Organic Aerosol in the Amazon, Science 31 (2012), 337, 1075-1078.

MAXYMUS - Reference guide for latest publications

Synchrotron Facility BESSY II



UE49 SMART | MPG

The high flux density beamline is specially designed for the high resolution spectromicroscope SMART. Located in a low-beta section with a round undulator source the PGM beamline illuminates the specimen surface in the SMART electron microscope with an ideal round beam with high flux density. The wide energy range of 100 to 1800 eV gives access to nearly all relevant XPS peaks and NEXAFS adsorption edges, used for chemical contrast in the photoemission electron microscope to study the local chemical composition on the surface in nanometer range. The variable choice of horizontal, vertical and (left/right) circular polarized light enables the investigation of *e.g.* molecular orientation in organic films or the magnetization in magnetic domains.

Instrument data

Location	9.2
Source	UE49
Monochromator	PGM
Energy range	100 - 1800 eV
Energy resolution	10000 at 200 eV
Flux	10^{11} - 10^{13} ph/s/300 mA
Polarization	Variable (linear and circular)
Divergence horizontal	11 mrad at specimen
Divergence vertical	11 mrad at specimen
Focus size (hor. x vert.)	10 µm x 5 µm on specimen surface
Distance Focus/last valve	350 mm
Height Focus/floor level	1350 mm
Free photon beam available	No
Fixed end station	Yes
Instrument responsible	Dr. Thomas Schmidt, thomas.schmidt@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

UE49 SMART - Reference guide for latest publications

SMART | MPG

Spectro-Microscopy with aberration correction for many relevant techniques

The instrument is an aberration corrected photo-emission electron microscope equipped with an imaging energy analyzer and installed at the high flux density beamline UE49 SMART. The SMART microscope is the first PEEM, showing successfully the simultaneous compensation for spherical and chromatic aberrations, enabling an outstanding lateral resolution of 2.6 nm (LEEM) and 18 nm (energy filtered XPEEM using W4f XPS peak) together with an increase in transmission by a factor of 6, demonstrated under experimental conditions at BESSY II. The multitude of operation modes – microscopy, spectroscopy and diffraction of photo-emitted and reflected electrons – and the variety of methods, *e.g.* photoemission electron microscopy (PEEM), energy-filtered XPEEM, NEXAFS-PEEM, LEEM, NEXAFS, XPS, UPS, XMCD, XMLD, photoelectron diffraction (PED), valence band structure mapping, and LEED, allow for a comprehensive characterization of inhomogeneous surfaces and thin films on nanometer scale with a surface sensitivity of only a few atomic layers. Examples are the local chemical composition of metal nano-particles and of structural domains in thin oxide films, the local molecular orientation of inhomogeneous organic films and local band structure measurements of ordered silica films.

Furthermore, the fast direct (*i.e.* non-scanning) imaging combined with the possibilities to deposit material on the specimen surface in measurement position, to cool or anneal the sample and to expose the surface to reactive gases during operation enable the *in-situ* and real time study of complex processes like *e.g.* film growth, alloying, chemical surface reaction, thermal desorption or phase transition on nanometer scale in video rate with chemical and structural contrast.

Instrument application

- Thin film growth (metal film, organic layers, thin oxide film)
- Metal nanoparticle
- Surface reactions
- Catalysis
- Phase transition
- Magnetic domains

References / Latest publications

[1] Schmidt, T. *et al.*: First experimental proof for aberration correction in XPEEM: Resolution, transmission enhancement, and limitation by space charge effects, Ultramicroscopy 126 (2013) 23-32.

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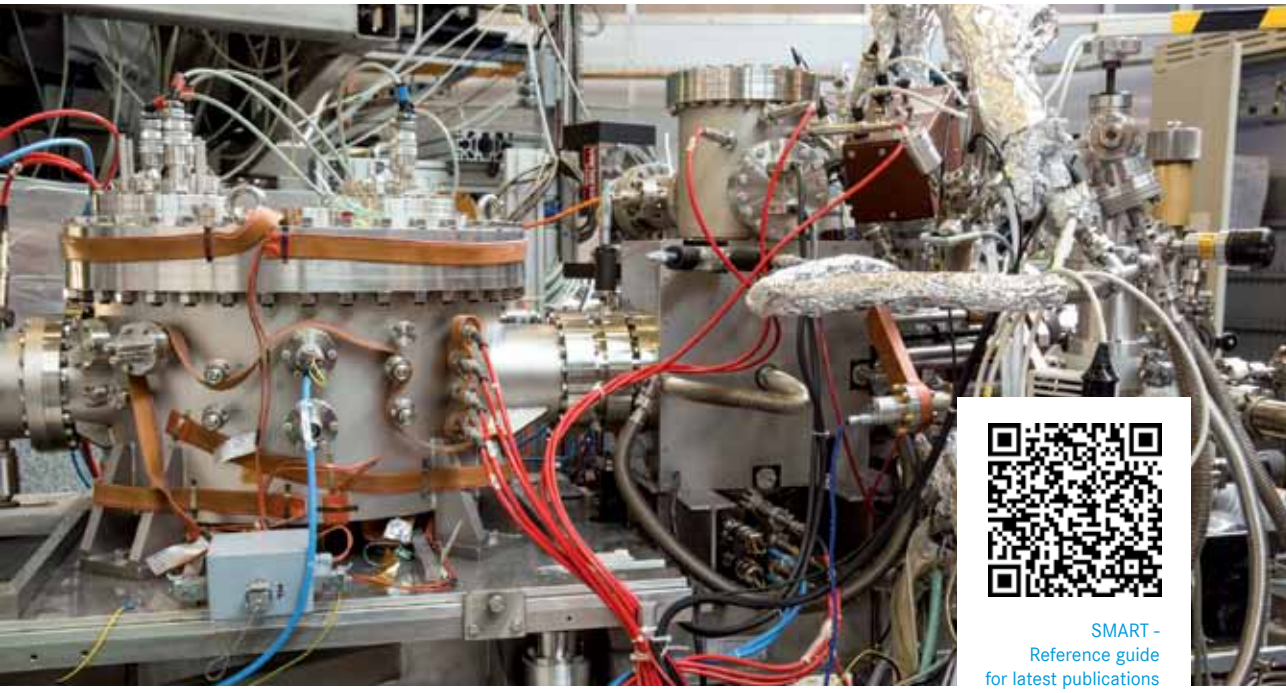


SMART - Reference guide for latest publications

Instrument data

Monochromator	PGM
Experiment in vacuum	Yes
Base pressure	10^{-10} mbar
Operation pressure	Up to 10^{-6} mbar
Temperature range	200 - 1800 K
No of ports pointing towards sample in operation position	8 (4 for evaporators)
Sample storage in UHV	6
Detector	Aberration corrected and energy-filtered XPEEM/LEEM system
Manipulator	Special sample holder design
Temperature measurement	W/Re thermocouple or pyrometer
Modes of operation/methods	• Microscopy: Photoelectron EM (PEEM), energy-filtered XPEEM, NEXAFS-PEEM, LEEM, Hg-PEEM • Spectroscopy: NEXAFS, XPS, UPS, Angular-resolved PES, XMCD, XMLD • Diffraction/angular distribution: Photoelectron Diffraction (PED), Valence band structure mapping, LEED
Lateral Resolution	• 2.6 nm (LEEM) • 18 nm (energy filtered XPEEM)
Energy resolution (XPEEM)	180 meV
Instrument responsible	Dr. Thomas Schmidt, thomas.schmidt@helmholtz-berlin.de

UE56-1 SGM | FZJ

Soft X-ray beamline with variable polarization

This beamline, built and operated by Forschungszentrum Jülich, is mainly used for it's fixed endstation, Jülich's aberation corrected LEEM/PEEM microscope. An apple-type undulator (period length 56 mm, „UE56", same as for the ZPM and PGM) generates the X-rays of linear vertical, linear horizontal or elliptical polarization. The optics include a spherical grating monochromator (SGM) with five interchangeable gratings to optimally cover a wide energy range. The refocusing optics, consisting of two bendable mirrors, enable the adjustment of the spot size: when working with a small field of view in the microscope, the focus is adjusted to the minimum, while the spot can be enlarged for survey pictures. Compared to other beamlines, all reflection angles are slightly more grazing which gains a good photon flux at higher photon energies, while this induces a poor second order suppression at the C-K-edge.

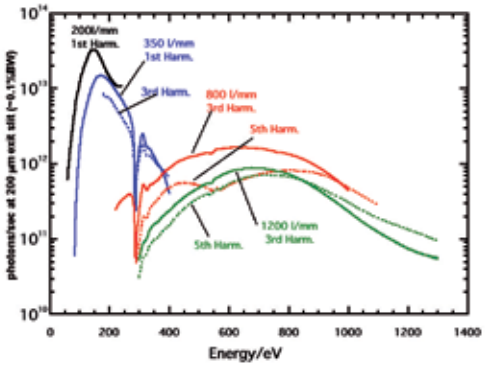
As an extra, an XMCD-chamber has been integrated into the beamline for a quick characterization of samples by NEXAFS / XMCD (RT, +/-0.5 T), independant from the PEEM.

Instrument data

Location	12.2
Source	UE56-1
Monochromator	SGM
Energy range	55 - 1500 eV
Energy resolution	> 10000
Flux	$2 \cdot 10^{13}$
Polarisation	• Horizontal • Vertical • Circular
Divergence horizontal	4 mrad
Divergence vertical	0.5 mrad
Focus size (hor. x vert.)	40 x 40 μm^2
Distance Focus/last valve	800 mm
Height Focus/floor level	1050 mm
Free photon beam available	No
Fixed end station	No
Instrument responsible	Dr. Stefan Cramm, FZ-Jülich, s.cramm@fz-juelich.de Dr. Slavomir Nemsak, FZ-Jülich, s.nemsak@fz-juelich.de

Instrument application

- Photoelectron microscopy (XPEEM)
- Electronic properties of thin films and single crystals
- Absorption spectroscopy (NEXAFS)
- Circular and linear X-ray Dichrosism (XMCD, XMLD)
- Ferroelectric and ferromagnetic domain images
- Magnetisation dynamics



EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

References / Latest publications

[1] Nickel, F. *et al.*: Time-resolved magnetic imaging in an aberration-cor-rected, energy-filtered photoemission electron microscope, Ultramicroscopy 130 (2013), 5462.

[2] Schaab, J. *et al.*: Imaging and characterization of conducting ferroelectric domain walls by photoemission electron microscopy, Applied Physics Letters 104 (2014), 232904.

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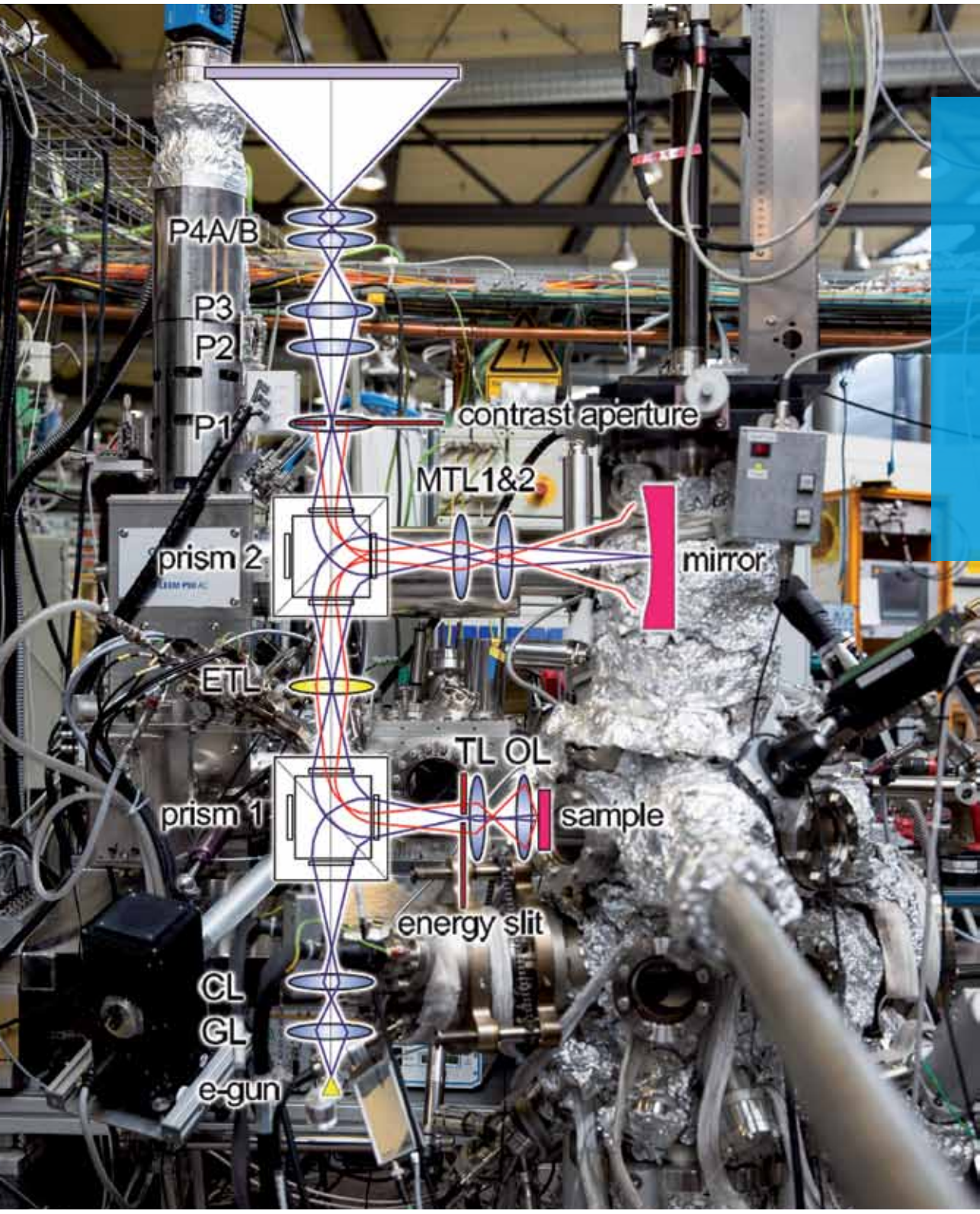
UE56-1 SGM - Reference guide for latest publications

Synchrotron Facility BESSY II



LEEM-PEEM | FZJ

Low-Energy- / Photoemission-Electron-Microscope

This microscope, operated stationary at the UE56/1-SGM beamline by Forschungszentrum Jülich, is equipped with a new state-of-the-art aberration corrector, minimizing electron-optical imperfections, allowing for higher instrument transmission and simultaneously better spatial resolution. In LEEM-Mode, electrons from a field-emission gun are reflected at the sample and a resolution below 5 nm has been demonstrated. Additionallly LEED patterns of small areas can be made visible. With soft X-rays (XPEEM), element-specific images are obtained by tuning the photon energy to particular absorption edges. At the same time, we get absorption spectra (NEXAFS, XMLD) of small regions of interest. Doing this with circular polarized X-rays we get an image of magnetic domains and XMCD-spectra. A pulsed excitation allows to perform stroboscopic XPEEM experiments for magnetization dynamics.

Instrument application

- Electronic properties of thin films and single crystals
- Micro - NEXAFS and X-ray Dichroism
- Ferroelectric and ferromagnetic domain images
- Magnetisation dynamics, currently sub-ns range

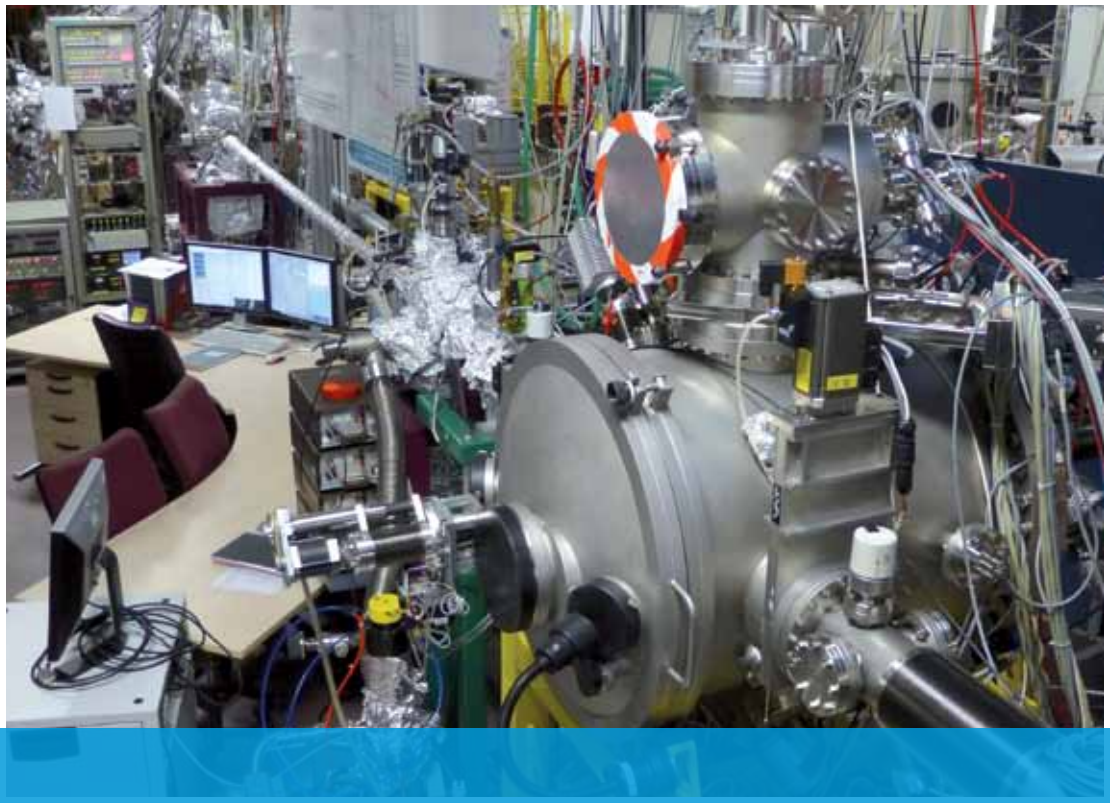
References / Latest publications

Please refer to the references of UE56-1 SGM

Instrument data

Monochromator	Spherical grating
Experiment in vacuum	Yes
Temperature range	150 -1600 K
Detector	Two-stage MCP (Hamamatsu)
Manipulators	5-Axis Piezo-contolled
Spatial resolution LEEM-mode	2 nm
Spatial resolution PEEM-mode	20 nm
base pressure	$4E^{-10}$ mbar
Preparation chamber	• Sputtering up to 1.5kV • Sample temperature range 300 - 1200 K • Pyrometric temp. measurement • LEED • Auger • Gas inlets: Ar, O_2, user specific • Base pressure 10^{-10} mbar
Instrument responsible	Dr. Slavomir Nemsak, FZ-Jülich, s.nemsak@fz-juelich.de Dr. Stefan Cramm, FZ-Jülich, s.cramm@fz-juelich.de

LEEM-PEEM - Reference guide for latest publications



D71 | PTB
Four-Crystal Monochromator Beamline

The PTB four-crystal monochromator beamline covers the photon energy range from 1.75 keV to 10 keV by using sets of four Si(111) and four InSb(111) crystals which can be interchanged under vacuum. Thus the K absorption edges of elements like silicon, phosphor, sulfur and chlorine are accessible which are relevant in technology and biology. The beamline provides radiation of very high spectral purity (higher order contamination typically below 10^{-4}) which is required for high-accuracy detector calibration with relative uncertainties below 1%. An X-ray reflectometer featuring all six degrees of freedom for sample alignment and several detectors like semiconductor photodiodes and energy-dispersive counting detectors is almost permanently installed. A large area (179 mm x 169 mm) vacuum compatible PILATUS 1 M hybrid-pixel detector is also available. A side branch of the beamline is the X-ray pencil beam facility (XPBF) which is used by the European Space Agency (ESA) to characterize silicon pore optics for future X-ray observatories.

The beamline is only accessible in the framework of cooperation projects with PTB.
Also available are the PTB beamlines U49-1 PTB compton (Roman Klein, roman.klein@ptb.de) and D71 PTB undispersed (Reiner Thornagel, reiner.thornagel@ptb.de).

Instrument data

Location	PTB laboratory at BESSY II
Source	D71
Monochromator type	Four-crystal monochromator
Monochromator crystals	Si(111) and InSb(111)
Energy range	1.75 keV to 10 keV
Energy resolution	< 1 eV
Flux	10^{10} s^{-1} to 10^{11} s^{-1}
Polarization	Horizontal
Divergence horizontal	< 2 mrad
Divergence vertical	< 0.3 mrad
Focus size	0.3 mm x 0.3 mm (hor. x vert.)
Height focus above floor level	1602 mm
Fixed end station	X-ray reflectometer
Instrument responsible	Dr. Michael Krumrey, michael.krumrey@ptb.de

EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

FIXED STATIONS CRG BESSY II

D71 - PTB-Xray - Reference guide for latest publications

Instrument application

- High-accuracy detector calibration
- Characterization of X-ray optical components
- Thickness determination of nanolayers with X-ray reflectometry (XRR)
- Size determination of nanoparticles with small-angle X-ray scattering (SAXS)
- Characterization of nanostructured surfaces with grazing incidence SAXS (GISAXS).

References / Latest publications

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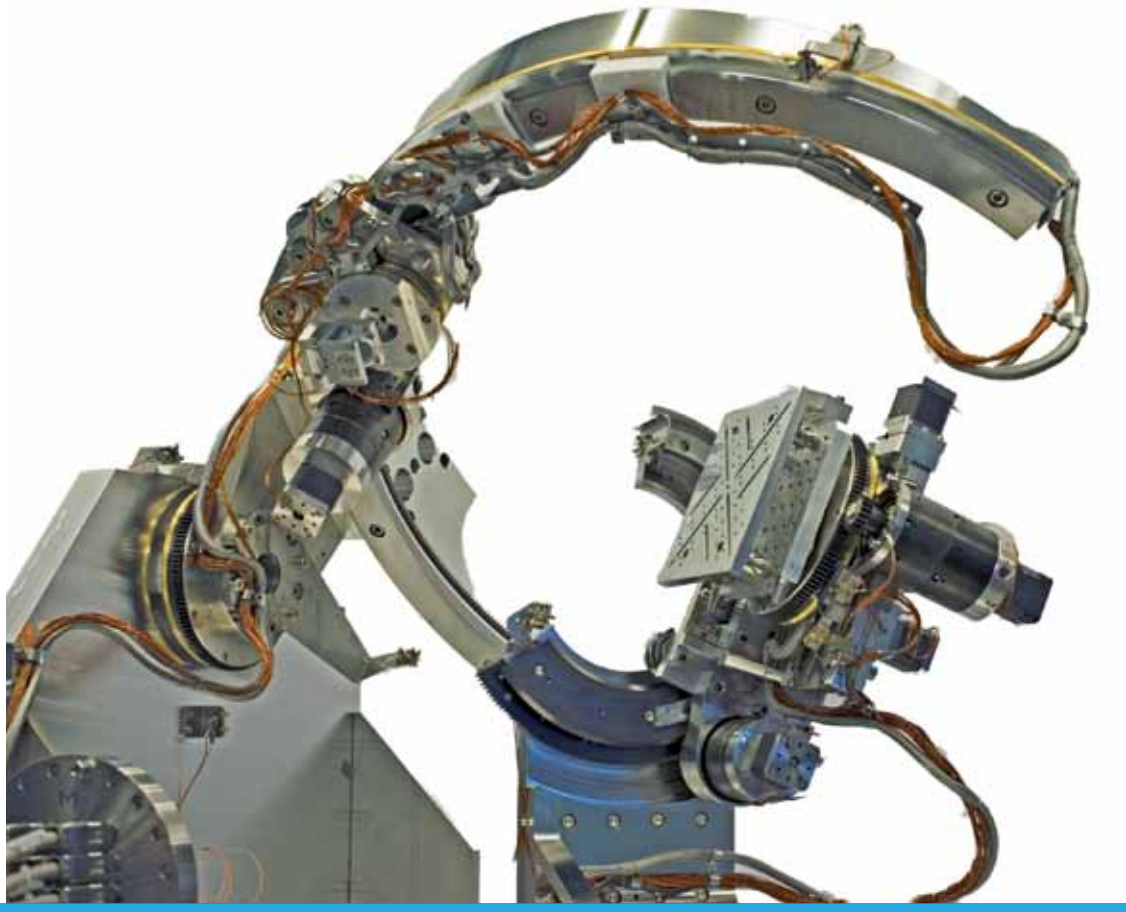

D72 | PTB
Soft X-ray Radiometry Beamline

The PTB soft X-ray radiometry beamline covers the photon energy range from 50 eV to 1800 eV using a PGM-type monochromator with a 1200-line/mm grating. The beamline is optimized to provide radiation of high spectral purity (higher order contamination typically of the order of 10^{-3} or lower) which is required for high-accuracy detector calibration with relative uncertainties below 1%. The beamline end-station is an EUV Ellipso-Scatteromter which allows for an arbitrary orientation of the plane of deflection with respect to the incoming linearly polarized beam. Samples up to (190 x 190 x 70) mm^3 and 5 kg weight can be accommodated. The option of a linear polarization analyzer also for the reflected beam exists.

The beamline is only accessible in the framework of cooperation projects with PTB.

Instrument application

- High-accuracy detector calibration
- Characterization of EUV and soft X-ray optical components
- Characterization of rough and nanostructured surfaces with EUV scatterometry.

Instrument data

Location	PTB laboratory at BESSY II
Source	D72
Monochromator type	Collimated plane grating monochromator
Monochromator grating	1200 lines/mm blazed
Energy range	50 eV to 1800 eV
Energy resolution	< 0.1 % relative bandwidth
Flux	10^{10} s^{-1} to 10^{11} s^{-1}
Polarization	Horizontal
Divergence horizontal	< 2 mrad
Divergence vertical	< 0.3 mrad
Spot size at experiment	Typically 0.3 mm x 1 mm (hor. x vert.)
Height experimental station above floor level	1820 mm
Fixed end station	EUV Ellipso-Scatterometer
Instrument responsible	Dr. Frank Scholze, frank.scholze@ptb.de

References / Latest publications

[1] Laubis, C. *et al.*: Status of EUV Reflectometry at PTB, Proc. SPIE 8679 (2013), 867921.

[2] Beckhoff, B. *et al.*: A quarter-century of metrology using synchrotron radiation by PTB in Berlin, Phys. Status Solidi B 246 (2009), 1415-1434.

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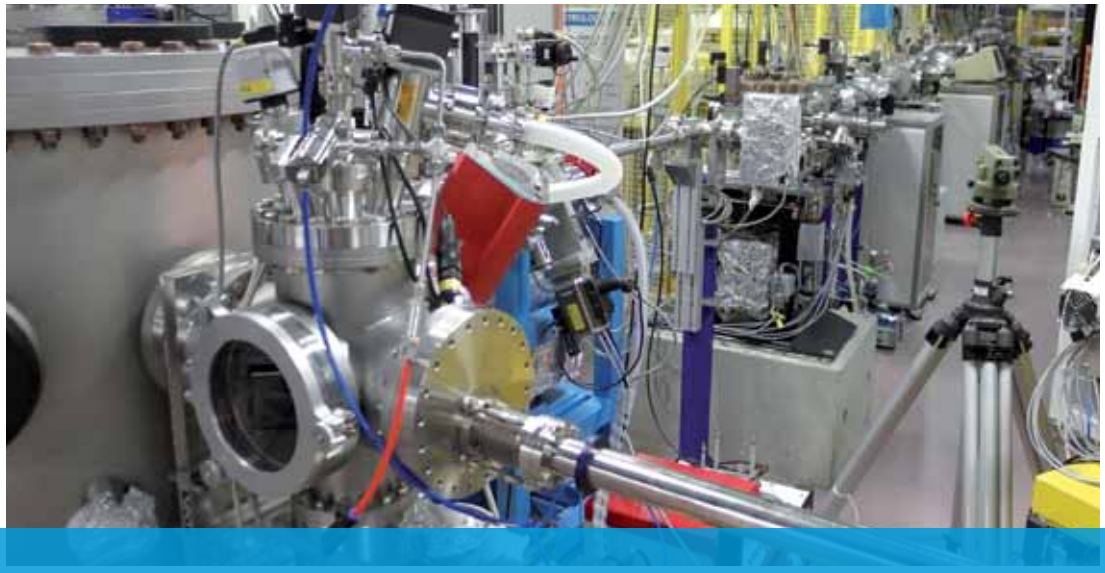
EXPERIMENTAL HALL BESSY II

BEAMLINES CRG BESSY II

FIXED STATIONS CRG BESSY II

D72 - PTB - Reference guide for latest publications



U49-1 | PTB
X-ray Spectrometer

The PTB plane-grating-monochromator beamline for undulator radiation provides a high photon flux with a high spectral purity within an energy range from 78 eV to 1860 eV. The radiant power output of the beamline well surpasses 5 µW in the parts of the accessible energy range. Due to optimized grating parameters such as the coatings, groove profile, line density and the total deviation angle, higher-order radiation contributions of less than 0.5% can be ensured for photon energies higher than 78 eV. The vertical focus size can be varied from 40 µm up to 600 µm, whereas the horizontal focus size is constantly 150 µm over the total energy range. Several instruments can be used at or up to 4 m behind the focus plane position of the beamline.

First, an ultra-high vacuum instrument enables various X-ray spectrometric techniques based on calibrated energy-dispersive X-ray detectors such as reference-free X-ray fluorescence analysis (XRF), total-reflection XRF, grazing-incidence XRF in addition to optional X-ray reflectometry measurements or polarization-dependent X-ray absorption fine structure analyses. With this instrument samples having a size of up to 100 mm x 100 mm can be analyzed with respect to their mass deposition, elemental, chemical or spatial composition. Key measurands are surface contamination, layer composition and thickness, depth profiles of matrix elements or implants, chemical binding states of nanolayers, nanoparticles or buried interfaces as well as the molecular orientation of bonds. Second, a calibrated wavelength-dispersive grating spectrometer provides moderate to high energy resolution in the soft X-ray range for X-ray Emission Spectrometry (XES) for light elements down to boron and transition metlas. An improved sensitivity using a single-bounce focusing optic enables the analysis and characterization of thin films down to the low nanometer range. The beamline is only accessible in the framework of cooperation projects with PTB.

Instrument data

Location	PTB laboratory at BESSY II
Source	U49-1
Monochromator type	Plane-grating monochromator
Energy range	78 eV to 1860 eV
Energy resolution	1000 to 8000
Flux	10^{8} s^{-1} to 10^{11} s^{-1}
Polarization	Horizontal
Divergence horizontal	< 0.6 mrad
Divergence vertical	< 0.4 mrad
Focus size	0.15 mm x 0.04 mm to 0.6 mm (hor. x vert.)
Height focus above floor level	1602 mm
Fixed end station	No, but three different UHV instrumentations for X-ray spectrometry at samples from 5 mm to 300 mm size
Instrument responsible	Dr. Burkhard Beckhoff, burkhard.beckhoff@ptb.de

Instrument application

- Reference-free quantification of X-ray Fluorescence (XRF) analysis
- Surface analysis by Total-reflection X-ray Fluorescence (TXRF)
- Characterization of nanolayered systems using Grazing Incidence X-ray Fluorescence (GIXRF) in combination with X-ray Reflectrometry (XRR) as well as Near Edge X-ray Absorption Fine Structure (NEXAFS)
- X-ray Emission Spectrometry (XES)

U49-1 PTB-XRS - Reference guide for latest publications

References / Latest publications

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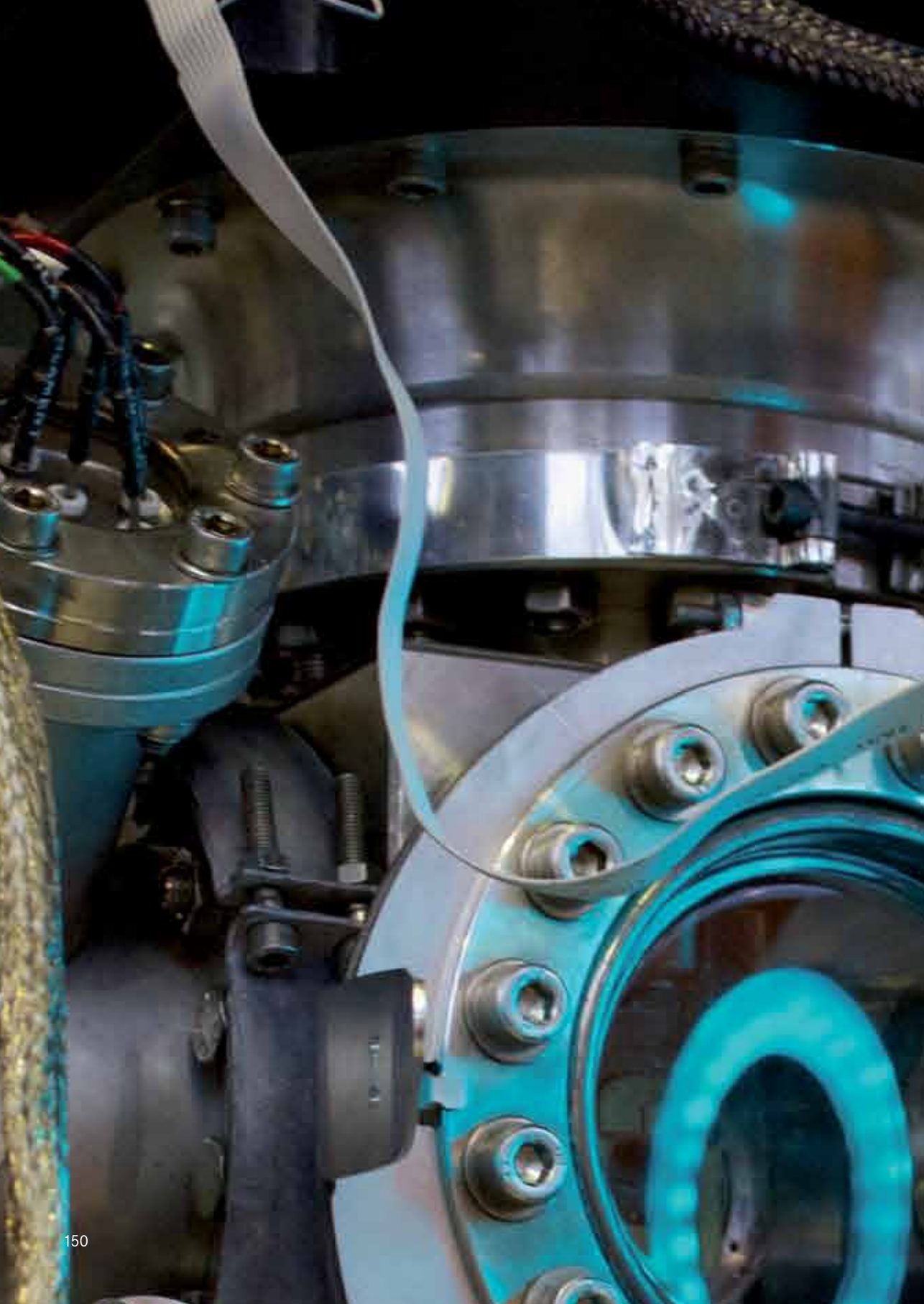


HZB Helmholtz Zentrum Berlin

BESSY II

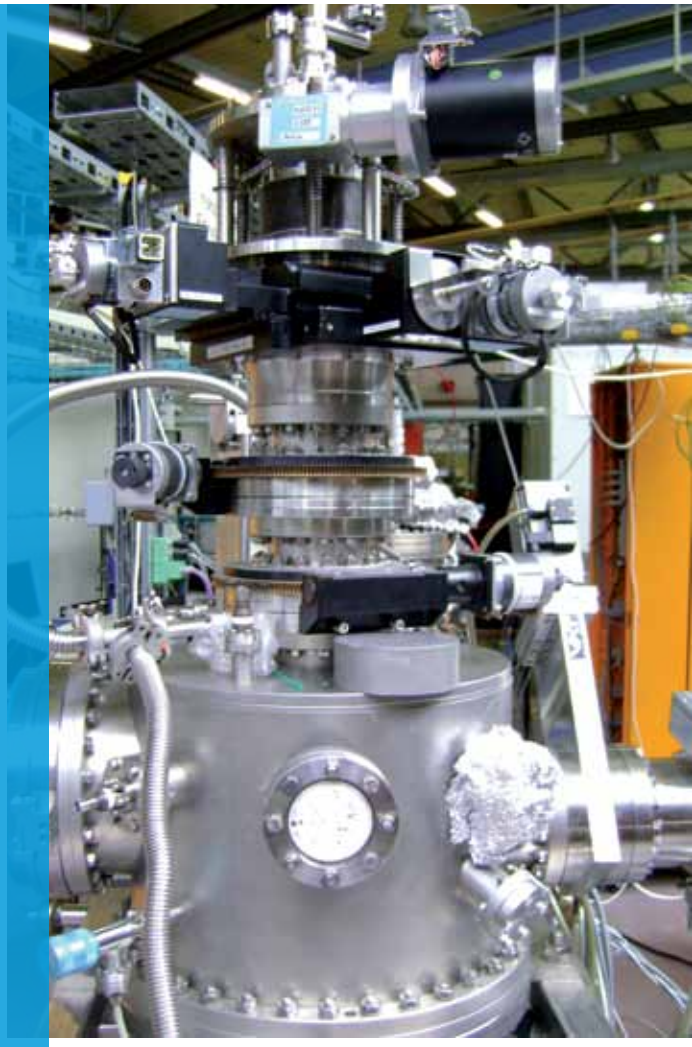
Flexible Stations

ALICE | Diffractometer for soft X-ray resonant magnetic scattering

The ALICE chamber was built as a diffractometer/reflectometer for XRMS applications and is in operation since December 2002. It combines a two-circle goniometer with an accessible range of 175° in 2θ. A magnetic field of ±7.1 kOe is available with a yoke that can rotate freely within the horizontal scattering plane. The whole chamber is mounted on a support frame and can thus be moved to various places (undulator or dipole beamlines) within the experimental hall, depending on the requirements of the experiment and beamtime allocation.

The sample holders are mounted on a cold-finger of a Janis flow cryostat that can be run with both LN_2 or LHe, where in the latter case temperatures down to 4 K can be reached.

Different sample holders can be accommodated on the sample manipulator. In the most common situation the samples are fixed vertically, perpendicular to the scattering plane and can rotate in the X-ray beam from normal to grazing incidence. Use of different signal channels is provided, including Total Electron Yield (TEY), Florescence Yield (FY), photo-diode (PD), and avalanche detector for XRMS. Depending on the sample holder used, different detector signals can also be measured simultaneously.



Instrument application / Samples

1. Single films
2. Multilayers
3. Bulk samples

Measurements:

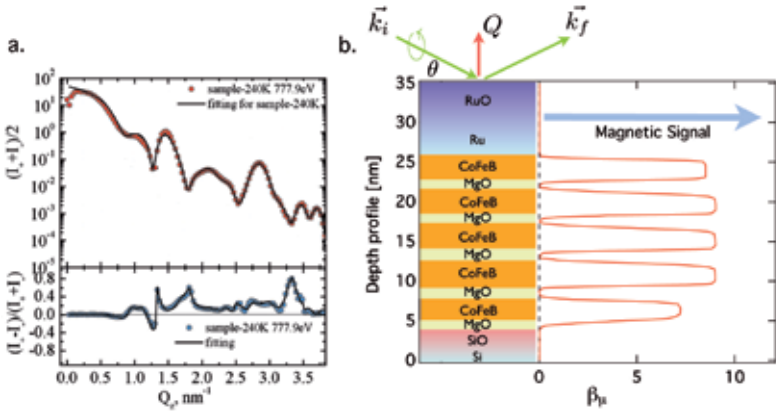
1. Spectroscopy (TEY, TR, FY, XMCD, XMLD)
2. Scattering (XRMS, Speckles)
3. Holography

Experiments:

Static
Dynamic (pump-probe)

Instrument data

Monochromator	Available at: dipole beamlines and undulator beamlines
Scattering Plane	Horizontal
Experiment in Vacuum	5x10^{7} mbar
Temperature range	4 - 470 K
Angular resolution	0.005 deg
Detector slit	30 µm - 2 mm
Magnetic field	Up to 0.7 T
Detectors	Si diode & APD diodes
Manipulator	Motorized XYZ XY resolution 1 µm Z resolution 0.01 mm Janis cryostat
Samples	Multilayers, single films, bulk materials, solid samples, Al membranes, SiN membranes
Instrument responsible	Dr. Radu-Marius Abrudan, radu-marius.abrudan@helmholtz-berlin.de



Reflectivity, magnetic asymmetry and magnetic profile of a CoFeB/MgO multilayer system.

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS CRG BESSY II

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ALICE - Reference guide for latest publications

CISSY | CIS - diagnostic using synchrotron radiation

Preparation and surface and interface analysis of thin film solar cell components using laboratory sources and synchrotron radiation.
In the CISSY end station, some of the crucial steps of the preparation of thin film solar cells can be performed in-system, allowing the direct transfer from preparation to the analysis chamber, avoiding contamination. Industrial preparation methods like magnetron sputtering (for transparent window layers) or the ILGAR process, which was developed at the HZB, as well as various wet chemical deposition methods (for buffer layers between the absorbing solar cells based on materials and window layers) are available.

Two spectrometers are used for analysis: A surface-sensitive photoelectron spectrometer (PES) (information depth of about 5 nm) and a much more bulk-sensitive X-ray emission spectrometer (XES) with a material-and energy dependent information depth of 60 to 500 nm. This allows the analysis of buried interfaces in layered systems, such as the buffer layer/absorber interface in chalcopyrite solar cells. Both methods allow detecting the presence and, to a certain degree, the concentration of elements in the sample based on their characteristic spectra. Furthermore, the chemical environment can also be determined, *i.e.* the oxidation state of the element in question and adjacent atomic binding partners may also be determined from the spectra. These highly sensitive instruments allow us to examine the processes involved in the manufacturing of thin film solar cells and also to investigate possible degradation mechanisms. Using the directly connected preparation modules, it is possible to stepwise build and analyze layer systems without transporting the sample through air and contaminating it.

Instrument data

Monochromator	Flexible
Experiment in vacuum	Yes
Temperature range	100-500 K
Detector	CLAM 4 hemispherical electron analyzer, XES-300 X-ray spectrometer
Manipulators	PINK x,y,z, rotation, tilt, heating and cooling
Preparation	Wet chemistry in glove box, sputter-depositon of oxides and other compounds
Instrument responsible	Dr. Iver Lauermann, iver.lauermann@helmholtz-berlin.de

Instrument application

- Analysis of surface and near surface elemental composition by soft X-ray PES (conductive inorganic or organic materials)
- Determination of surface chemistry (oxidation states)
- Analysis of band line-up in semiconductor multilayers
- Bulk analysis by XAS and XES
- In-system preparation of oxididic and sulfidic thin layers

References / Latest publications

[1] Sarmiento-Pérez, R. *et al.*: Band alignment and local structure of CIGS alloys from combining X-ray absorption spectroscopy and ab initio calculations, submitted to Applied Physics Letters (2014).

[2] Merdes, S. *et al.*: Zn(O,S) buffer prepared by atomic layer deposition for sequentially grown $Cu(In,Ga)(Se,S)_2$ solar cells and modules, Solar Energy Materials & Solar Cells, 126 (2014),120-124.

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EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

CISSY - Reference guide for latest publications

FEMTOSPEX Magnetism | Experimental station for fs time resolved XMCD and XAS

The FEMTOSPEX XMCD/XAS experimental station was set up in 2004 for the proof-of-principle Femtoslicing experiments and has since then been a workhorse for both in-house research and user operation at the HZB. It has been built particularly for time-resolved XAS and XMCD measurements in transmission, coping with the reduced photon flux in fs time resolved experiments. The main scientific focus is on ultrafast magnetization dynamics and time-resolved X-ray absorption spectroscopy.

The experimental setup for laser pump – X-ray probe on magnetic samples consists of a measurement chamber housing the magnet and transmission sample, and the detector chamber with a fast avalanche photodiode (APD). To preserve the femtosecond time resolution the laser and X-ray beams enter through the beamline flange in a collinear geometry. An Al foil mounted between the chambers prevents laser light to enter the detection chamber with the APD.

EXPERIMENTAL HALL BESSY II

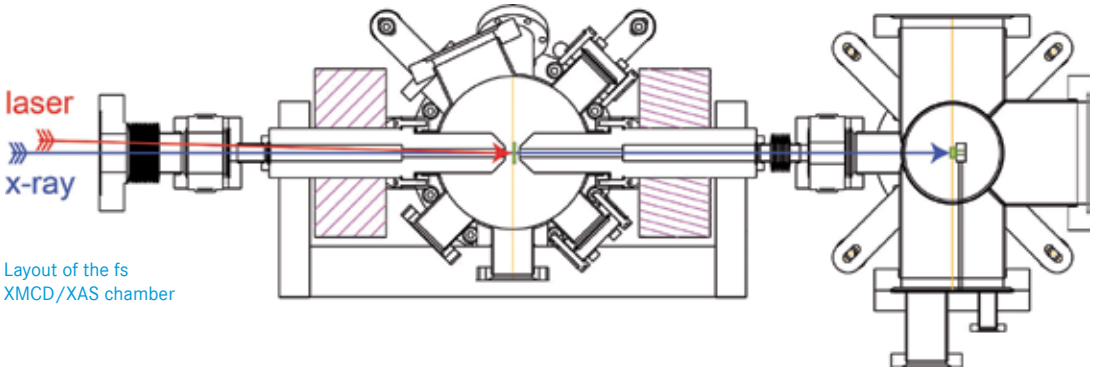
FLEXIBLE STATIONS BESSY II

Instrument data

Monochromator	Soft X-ray and FEMTOSPEX
Experiment in vacuum	Yes
Temperature range	30 - 450 K (low-T), 130 - 750 K (variable T)
Detector	GaAs Photodiode, gated Avalanche Photodiode (1 ns)
Manipulators	Low-Temprerature (He) cryostat, variable temperature cryostat
Magnetic field (longitudinal)	0.5 Tesla
Magnetic field (transverse)	0.04 Tesla
Instrument responsible	Dr. Ilie Radu, ilie.radu@helmholtz-berlin.de Dr. Loic Le Guyader, loic.le_guyader@helmholtz-berlin.de

Instrument application

- Magnetization and Spin Dynamics
- Transient Electronic Structure
- Spin and Orbital Momentum Dynamics
- Ultrafast Magnetization Switching and Demagnetization
- Ultrafast Generation of Magnetism
- Ultrafast Spin Transport



Layout of the fs XMCD/XAS chamber

References / Latest publications

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[2] Boeglin, C. *et al.*: Distinguishing the ultrafast dynamics of spin and orbital moments in solids, Nature 465 (2010), 458-461.

[3] Eschenlohr, A. *et al.*: Ultrafast spin transport as key to femtosecond demagnetization, Nature Materials 12 (2013), 332-336.

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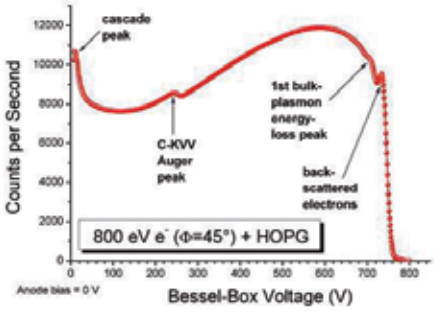
FEMTOSPEX Magnetism - Reference guide for latest publications

FEMTOSPEX Molecules and Surfaces | Electron spectroscopy setup for time resolved Laser-Pump/X-ray-probe experiments

An electron spectroscopy setup for time resolved Laser-Pump/X-ray-Probe -experiments is currently being built and in the test phase regarding reproducibility, detection solid-angle, efficiency, time resolution, energy resolution, spectrometer factor, and so on.

Instrument application

XMLD, time-resolved studies, EXAFS, NEXAFS, XMCD, angular-resolved PES, XPS, UPS



Test electron-spectrum for 800 eV primary electrons on HOPG, taken with a simple Faraday-cup detector.

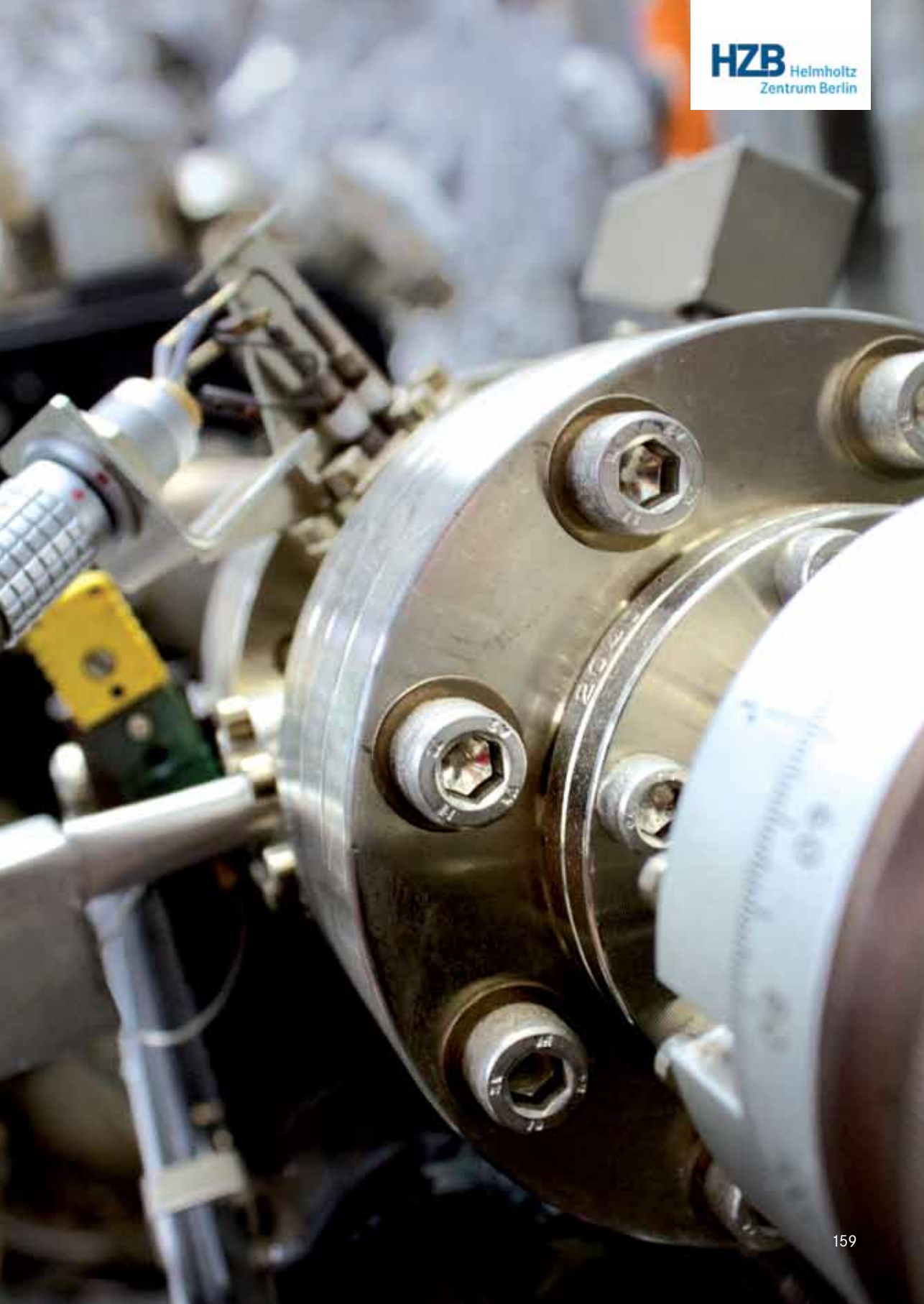
EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

FEMTOSPEX Molecules and Surfaces - Reference guide for latest publications

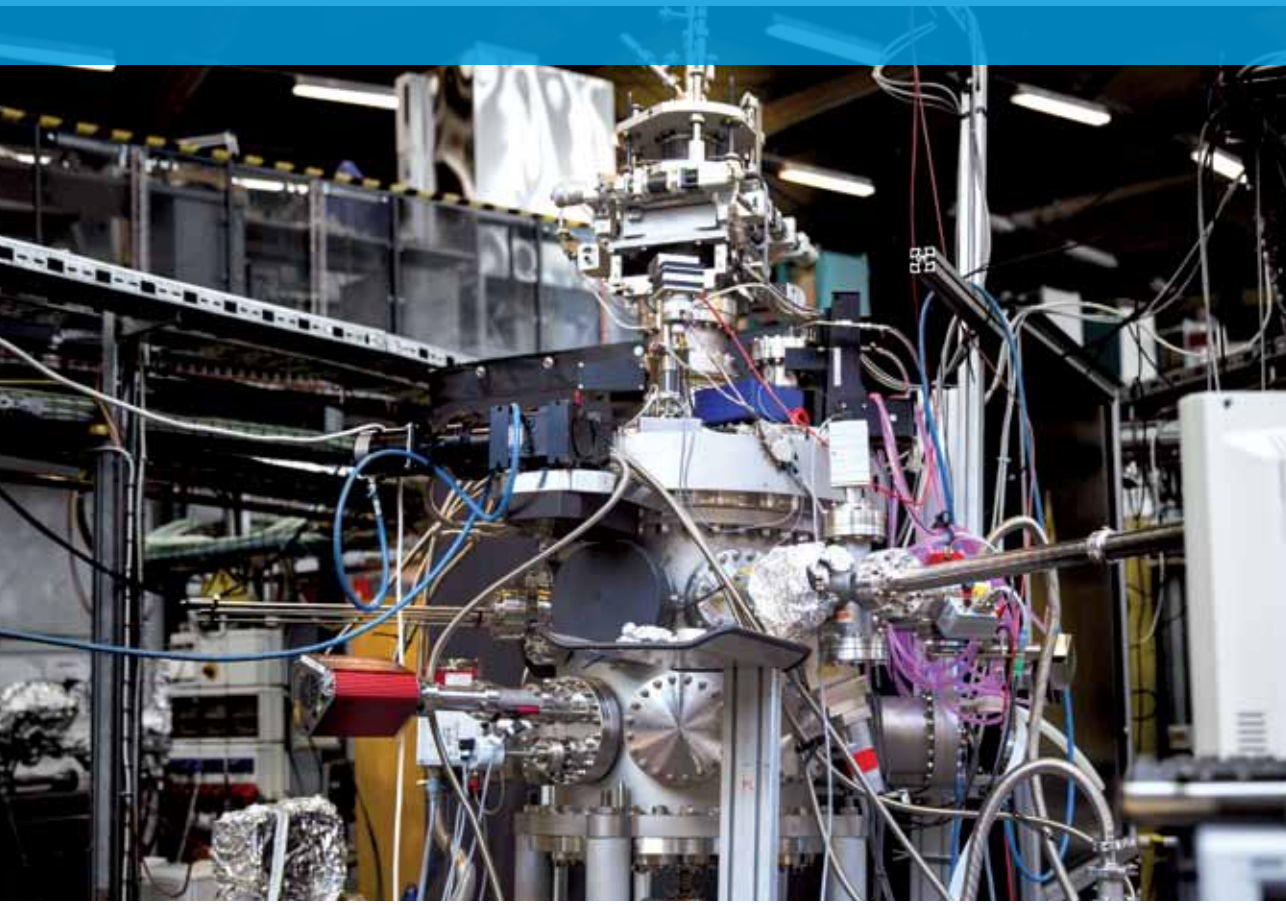
Instrument data

Monochromator	Soft X-ray
Experiment in vacuum	Yes
Detector	Bessel Box, ARTOF 2k
Instrument responsible	Dr. Florian Sorgenfrei, florian.sorgenfrei@helmholtz-berlin.de Prof. Dr. Gregor Schiwietz, schiwietz@helmholtz-berlin.de



FEMTOSPEX Scattering |
Time-resolved resonant soft X-ray diffraction

Within the last two decades resonant soft X-ray diffraction (RSXD) has emerged as a highly efficient experimental technique. It allows probing nanoscale ordering phenomena in solid state materials, like electronic order, charge or orbital order, as well as magnetic order. In particular, RSXD is one of the few methods that can probe antiferromagnetic order. For these reasons time-resolved pump probe RSXD is ideally suited to study the dynamics of photo-induced phase transitions in correlated materials when it is combined with ultra-short photon pulses. A special case of resonant X-ray diffraction is the spectroscopic measurement of the specular sample surface (single Bragg plane) reflection at grazing incidence angles (<12°). The advantage of X-ray reflection spectroscopy (XRS) over XAS in transmission geometry is that it lifts the strong constrain of having to use thin films of a few tens of nanometers thickness as a sample. This allows access to dynamics in crystalline bulk samples and films or nanostructures grown on thicker substrates.



EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

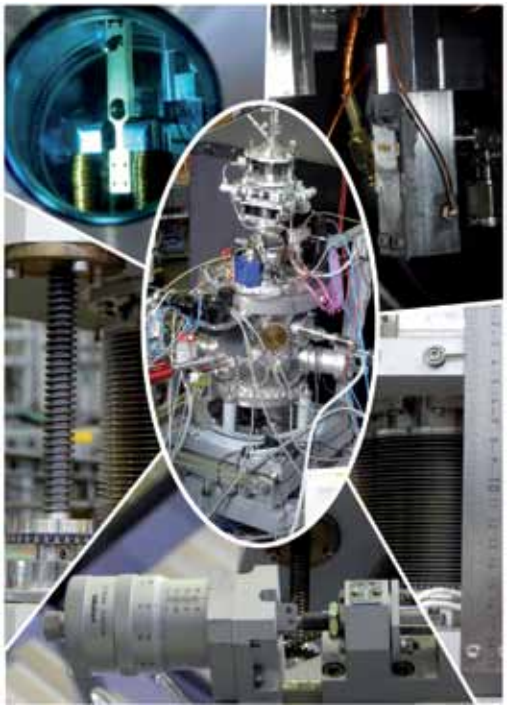
FEMTOSPEX Scattering - Reference guide for latest publications

Instrument data

Monochromator	Soft X-ray and FEMTOSPEX
Experiment in vacuum	Yes
Temperature range	6 - 400 K
Detector	Photon detection (see detection special features below)
Manipulators	x/y/z; two cycle goniometer
Sample environment	• *In-situ* sample cleaving available • Sample transfer system available • Measurements at cryogenic temperatures possible
Detection special features	• fs-laser synchronized gated detection (Avalanche Photo Diode) • Single photon counting detection for low intensity measurements • Laser light screened detection (>10^{12} attenuation) • Sample current measurement available • Data acquisition via SPEC
Diffractometer features	• Motor controlled two-circle goniometer • Software motion control via SPEC • Variable angular resolution
UHV	< 10^{-9} mbar (turbo-molecular pump, ion pump, LN-cooling trap)
Miscellaneous	Laser safety protected viewports
Instrument responsible	Dr. Niko Pontius, pontius@helmholtz-berlin.de Dr. Christian Schüßler-Langeheine, christian.schuessler@helmholtz-berlin.de

Instrument application

Since 2008 the RXD and more recently XRS have been made available for ultrafast studies at the FemtoSpeX Slicing Facility. A dedicated two circle UHV diffractometer has been set up for diffraction (reflection) geometries within the horizontal plane. By cryogenic cooling sample temperatures down to 6 K can be reached. Avalanche photodiodes (APDs) are used for gated photon pulse detection. The angular acceptance of the diffractometer is set by vertical detector entrance slits of variable size. The APDs are screened from light of the pump-laser by Al membranes (Luxel Corporation) and a light tight housing. Low noise amplification (ca. 60 dB by Hamamatsu and Kuhne preamplifiers) allows besides analog pulse detection for time-correlated single-photon pulse counting. Generally signals as low as ~5 photons/sec from the sample can be detected. This corresponds to a diffraction (reflection) efficiency of >$5 \cdot 10^{-5}$.



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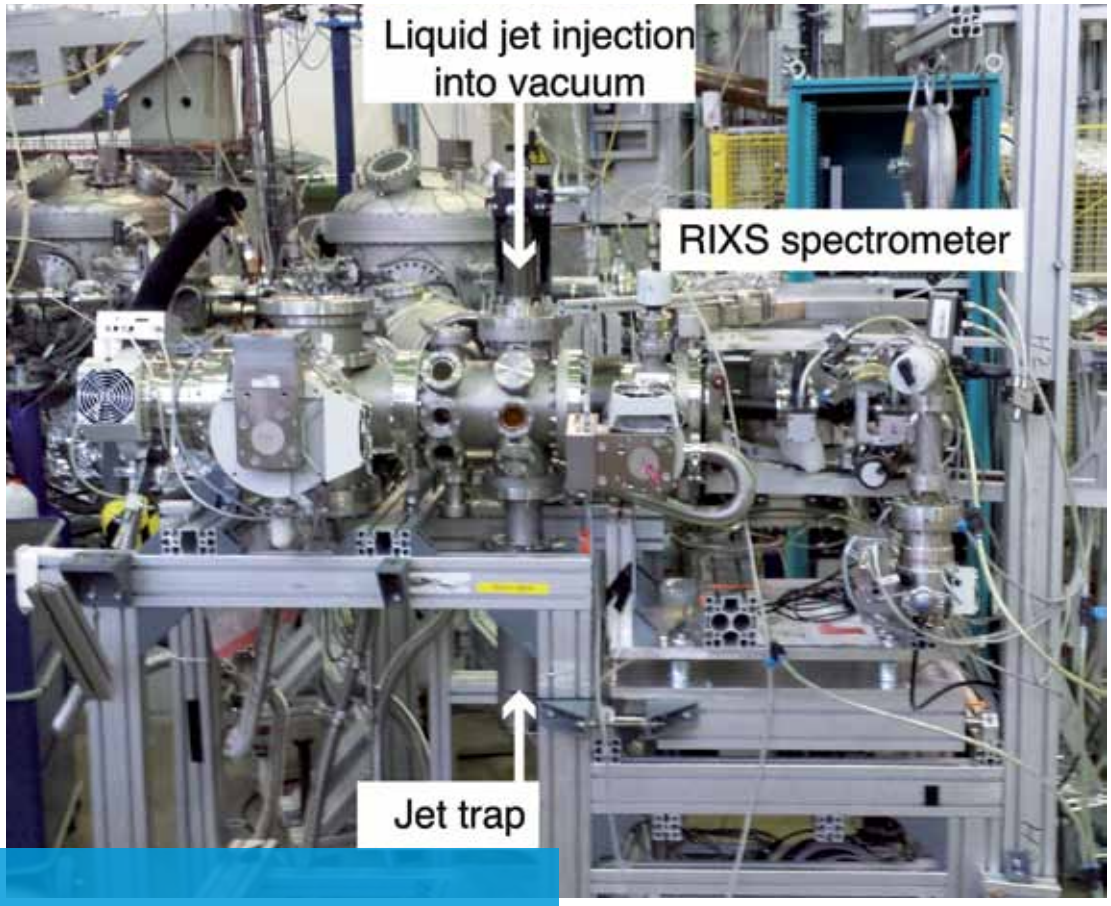

Liquid flexRIXS | RIXS end-station for molecular systems

Endstation for time-resolved and steady-state RIXS measurements on liquid and solid samples and for complementary use at FELs and at BESSY II. The RIXS spectrometer of the end station is a modified GRAZE IV (XES 350) with three gratings. These cover the range between 50 and 900 eV. The resolution amounts to approximately 40 meV at 50 eV and 0.7 eV at 900 eV. Total fluorescence yield absorption measurements with a photodiode or partial fluorescence yield absorption measurements with the spectrometer are possible. Liquid samples are prepared in vacuum as thin jets (diameter 5-30 µm). The jet freezes after passing the interaction region in a liquid nitrogen cooled trap. To protect the beam line from the typical 10^{-3} mbar range in the measurement chamber during liquid jet operation, three differential pumping stages are used. The MCP-based detector is protected by an X-ray transmissive yet vacuum-tight thin foil. Solids can be held in vacuum with standard manipulators (CF 100). Static and time resolved RIXS measurements at liquids and solids as well as non-linear processes are conducted with this experimental station at BESSY II and FELs. Depending on the X-ray spot size the jet speed in vacuum allows for refreshing the sample in the interaction region with MHz repetition rates. The apparatus is open to collaborative Research at BESSY II and FELs.

Instrument data

Energy range	Soft X-rays from 50 to around 900 eV
Resolving power	Better than 1000
Sample environment	Liquid jet in vacuum, three differential pumping stages towards the beam line, solid samples can be mounted on a CF 100 manipulator
Temperature range	Jet temperature can be controlled with a water jacket
Detectors	GaAs-Photodiode and RIXS spectrometer with MCP, phosphor and CCD
Samples	Liquid and solid
Instrument responsible	Dr. Annette Pietzsch, annette.pietzsch@helmholtz-berlin.de

Instrument application

- Static RIXS of liquids and liquid solutions of molecules at BESSY II
- Pump-probe RIXS of liquids and liquid solutions at FELs
- Static RIXS of solid samples at BESSY II
- Pump-probe RIXS of solid samples at FELs
- Investigation of non-linear X-ray induced processes at FELs
- Static and pump-probe fluorescence yield absorption at BESSY II and FELs

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

References / Latest publications

[1] Kunnus, K. *et al.*: A setup for resonant inelastic soft X-ray scattering on liquids at free electron laser light sources. Rev. Sci. Instrum. 83 (2012), 123109.

[2] Wernet, P. *et al.*: Dissecting Local Atomic and Intermolecular Interactions of Transition-Metal Ions in Solution with Selective X-ray Spectroscopy. J. Phys. Chem. Lett. 3 (2012), 3448-3453.

[3] Josefsson, I. *et al.*: Ab Initio Calculations of X-ray Spectra: Atomic Multiplet and Molecular Orbital Effects in a Multiconfigurational SCF Approach to the L-Edge Spectra of Transition Metal Complexes. J. Phys. Chem. Lett. 3 (2012), 3565-3570.

[4] Wernet, P. *et al.*: Mapping chemical bonding of reaction intermediates with femtosecond X-ray laser spectroscopy. EPJ Web of Conferences 41 (2013), 05025.

[5] Mitzner, R. *et al.*: L-Edge X-ray Absorption Spectroscopy of Dilute Systems Relevant to Metalloproteins Using an X-ray Free-Electron Laser. J. Phys. Chem. Lett. 4 (2013), 3641-3647.

Liquid flexRIXS-Reference guide for latest publications

Solid flexRIXS | Endstation for solid systems

Endstation for complementary application of RIXS, diffraction (resonant scattering) and absorption measurements both at BESSY II and free-electron lasers. This endstation is equipped with a two-axis rotatable sample holding manipulator (one axis motorized). The sample stage can be cooled with liquid Helium and in a different configuration also heated by electron bombardment heating to more than 1000 °C. Sample drain current can be measured for total electron yield absorption measurements and a photodiode (optionally with a biased mesh to repel electrons) can be used for diffraction / resonant scattering experiments as well as fluorescence yield detection. Furthermore, the endstation is equipped with a modified Grace IV / XES 350 spectrometer that can cover a photon energy range from 50 to above 900 eV. Resolving powers above 1000 have been shown to be easily achievable and can be furthered at the expense of count rate. The emission

is dispersed from three different gratings to cover the full energy range with optimal count rate. The dispersed light is detected by an MCP, phosphor screen, CCD combination. The system is completely software-controlled so that long macros can be used for extended measurement plans. The detectors can be made blind to optical radiation so that it can be used in pump-probe setups to study dynamics at BESSY II and FELs. Non-linear X-ray spectroscopy can be conducted with this setup as well. The chamber is open for collaborative research at BESSY II and FELs.

Instrument data

Energy Range	50 to above 900 eV
Resolving Power	Above 1000
Sample Environment	UHV for solid samples, controlled azimuth rotation
Temperature Range	From liquid Helium temperatures to above 1000°C
Detectors	GaAs and Si photodiodes optionally shielded by a biased mesh or light-tight metal filters, optically blind MCP-Phosphor-CCD combination behind the spectrometer
Samples	Solid
Instrument responsible	Dr. Martin Beye, martin.beye@helmholtz-berlin.de

Instrument application

- RIXS of correlated materials across phase transitions
- RIXS of catalyst materials
- Angle dependent fluorescence yield studies
- Soft X-ray resonant reflectivity measurements
- Pump-Probe RIXS experiments
- Pump-Probe fluorescence yield and scattering studies
- Non-linear X-ray spectroscopy

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

References / Latest publications

[1] Beye, M. *et al.*: Dynamics of Electron-Phonon Scattering: Crystal- and Angular-Momentum Transfer Probed by Resonant Inelastic X-ray Scattering, Phys. Rev. Lett. 103 (2009), 237401.

[2] Beye, M. *et al.*: Measurement of the predicted asymmetric closing behaviour of the band gap of silicon using X-ray absorption and emission spectroscopy, New J. Phys. 12 (2010), 043011.

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[4] Beye, M. *et al.*: Stimulated X-ray emission for materials science, Nature 501 (2013), 191-194.

Solid flexRIXS - Reference guide for latest publications

LiquidJet PES |
Soft X-ray Photoelectron Spectroscopy from Aqueous Solution

The LiquidJet PES apparatus is a specialized end-station for studying the electronic structure of liquid water, aqueous and non-aqueos solutions with soft X-ray photoemission spectroscopy. Liquid samples are introduced into the main interaction chamber via a 15-20 micrometer mircojet, forming a free liquid surface in vacuum. One 1500 l/s turbo pump and several LN_2 cold-traps keep the pressure on the 10^{-5} mbar level under operation conditions. Electrons are detected by a SPECS EA10 hemispherical analyzer with a 100-200 µm skimmer orifice, acting as a pressure barrier between main chamber and EA.

Instrument data

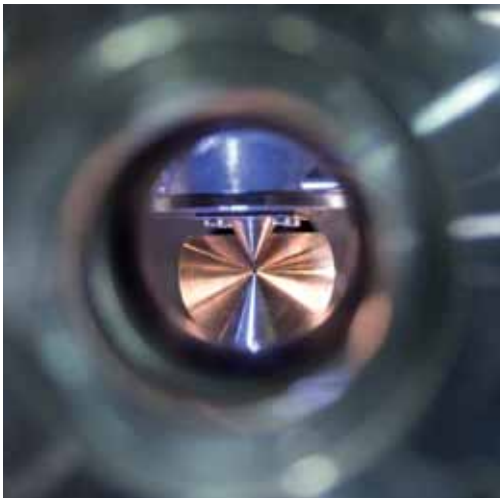
Monochromator	Designed to match layout of few beamlines
Experiment in vacuum	Yes
Temperatur range	275 - 300 K
Detector	SPECS EA10-MCP electron analyzer
Manipulators	xyz manipulators for positioning the liquid jet and the jet- catching reservoir
Mircojet Unit	Temperature-stabilized liquid microjet emerging from typically 15-20 micrometer diameter quartz capillaries
Instrument responsible	Dr. Bernd Winter, bernd.winter@helmholtz-berlin.de

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

Instrument application

- Systems: organic and inorganic molecules, and nanoparticles in water
- Electronic structure of liquid water and aqueous solution
- Solute and solvent electron binding energies
- Core-level chemical shifts, lowest ionization energies and reorganization energies
- Structure and composition of solution interfacial structure; depth profiles
- Chemical equilibria at the solution surface
- Ultrafast relaxation processes induced by core-level ionization/excitation
- Ultrafast energy and charge transfer in hydrogen-bonded systems
- Resonant and non-resonant autoionization (Auger) electron spectroscopy
- Electron scattering processes in water and in solution
- Angular-resolved PE spectroscopy from aqueous solution



References / Latest publications

[1] Thürmer, S. *et al.*: On the nature and origin of dicationic, charge-separated species formed in liquid water on X-ray irradiation, Nat Chem 5 (2013), 590-596.

[2] Thürmer, S. *et al.*: Photoelectron Angular Distributions from LiquidWater: Effects of Electron Scattering, Phys. Rev. Lett. 111 (2013), 173005.

[3] Thürmer, S. *et al.*: Relaxation of Electronically Excited Hydrogen Peroxide in Liquid Water: Insights from Auger-Electron Emission, J Phys Chem C 117 (2013), 22268-22275.

[4] Margarella, A. M. *et al.*: Dissociation of Sulfuric Acid in Aqueous Solution: Determination of the Photoelectron Spectral Fingerprints of H_2SO_4, HSO_4^-, and SO_4^{2-} in Water, J Phys Chem C 117 (2013) 8131-8137.

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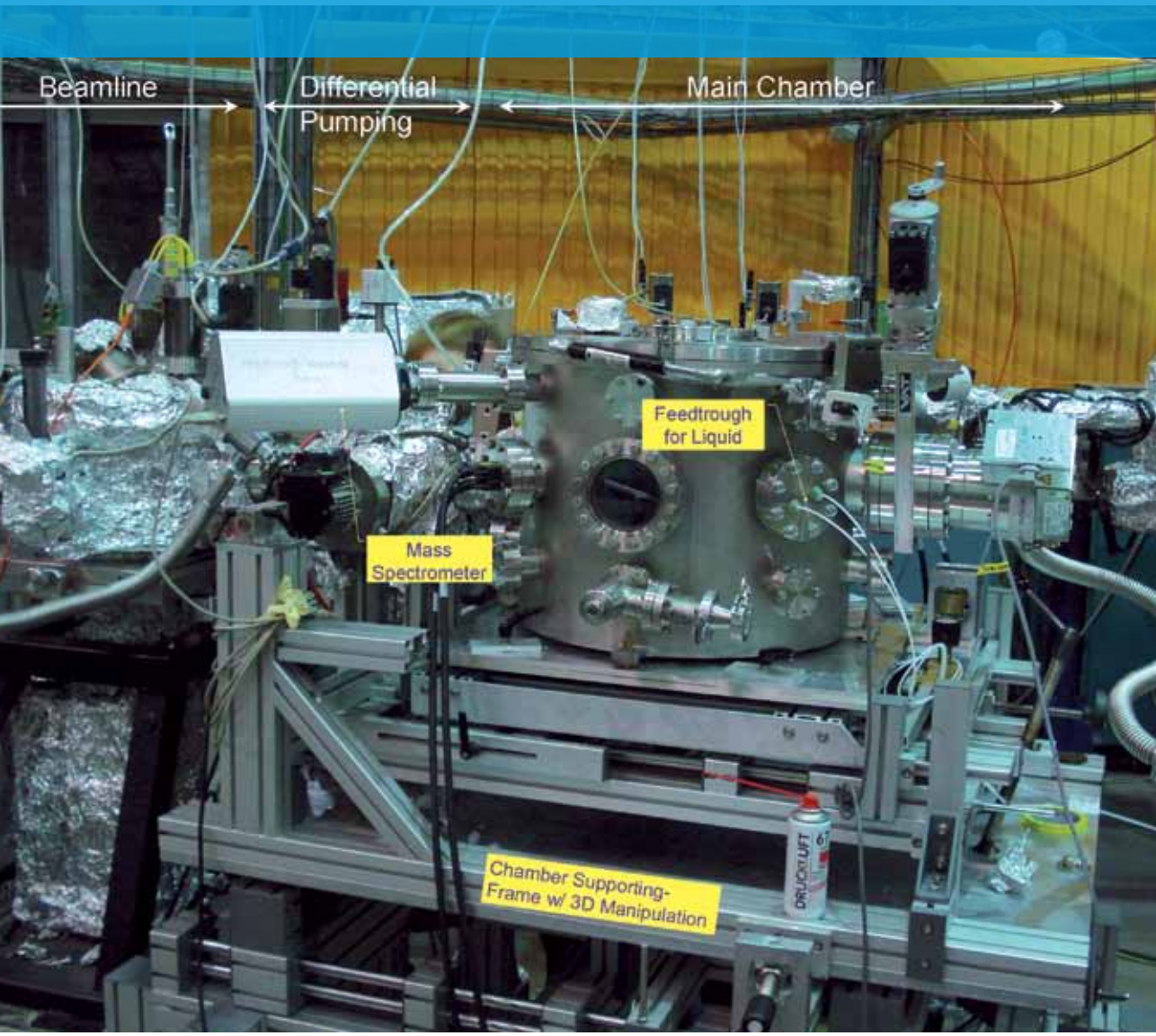
[6] Brown, M. A. *et al.*: Measure of Surface Potential at the Aqueous–Oxide Nanoparticle Interface by XPS from a Liquid Microjet, Nano Lett. 13 (2013), 5403-5407.

LiquidJet PES - Reference guide for latest publications

Liquidrom | Liquids and degassing samples equipment

Liquidrom is a vacuum system dedicated to X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) for liquid samples. The system is equipped with time-of-flight (TOF) electron energy analyzer and GaAs photodiode as electron and photon detectors respectively. Intense laser pulses, synchronized with the synchrotron X-ray pulses (only in single bunch mode), are often employed in Liquidrom system to excite (pump) samples by laser and successively (within nanoseconds) measure (probe) samples by X-ray in order to study the dynamic properties of various liquid phase molecules in strong laser field (Pump-Probe experiment).



Instrument data

Monochromator	None
Experiment in vacuum	Yes
Temperature range	283 – 373 K
Detector	Time-of-flight (TOF) electron energy analyzer, GaAs photodiode
Manipulators	Motorized XYZ sample manipulator with micrometer precision
Chamber pressure	10^{-5} mbar base pressure in main chamber and 10^{-8} mbar in TOF analyzer when liquidjet running in main chamber
Instrument responsible	Prof. Dr. Emad Flear Aziz, emad.aziz@helmholtz-berlin.de Jie Xiao, jie.xiao@helmholtz-berlin.de

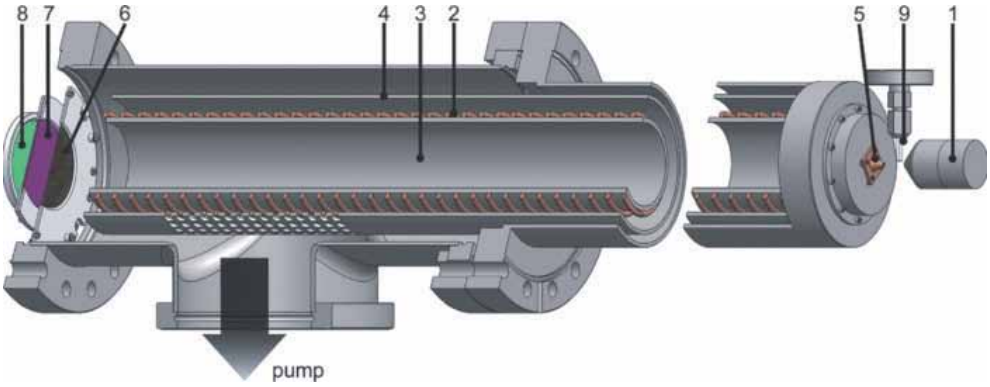
Instrument application

- Ultrafast molecular dynamics in liquid solution, *e.g.* solvated electron, Inter-atomic Coulombic decay (ICD).
- Electronic structure of liquid in strong laser field

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

Design of the TOF electron spectrometer:
(1) permanent magnet with a soft iron cone, (2) solenoid, (3) drift tube, (4) μ-metal shield, (5) skimmer of 500 μm size, (6) copper mesh, (7) double-stack of MCP, (8) fluorescence screen, and (9) nozzle to introduce the sample.



Liquidrom - Reference guide for latest publications

References / Latest publications

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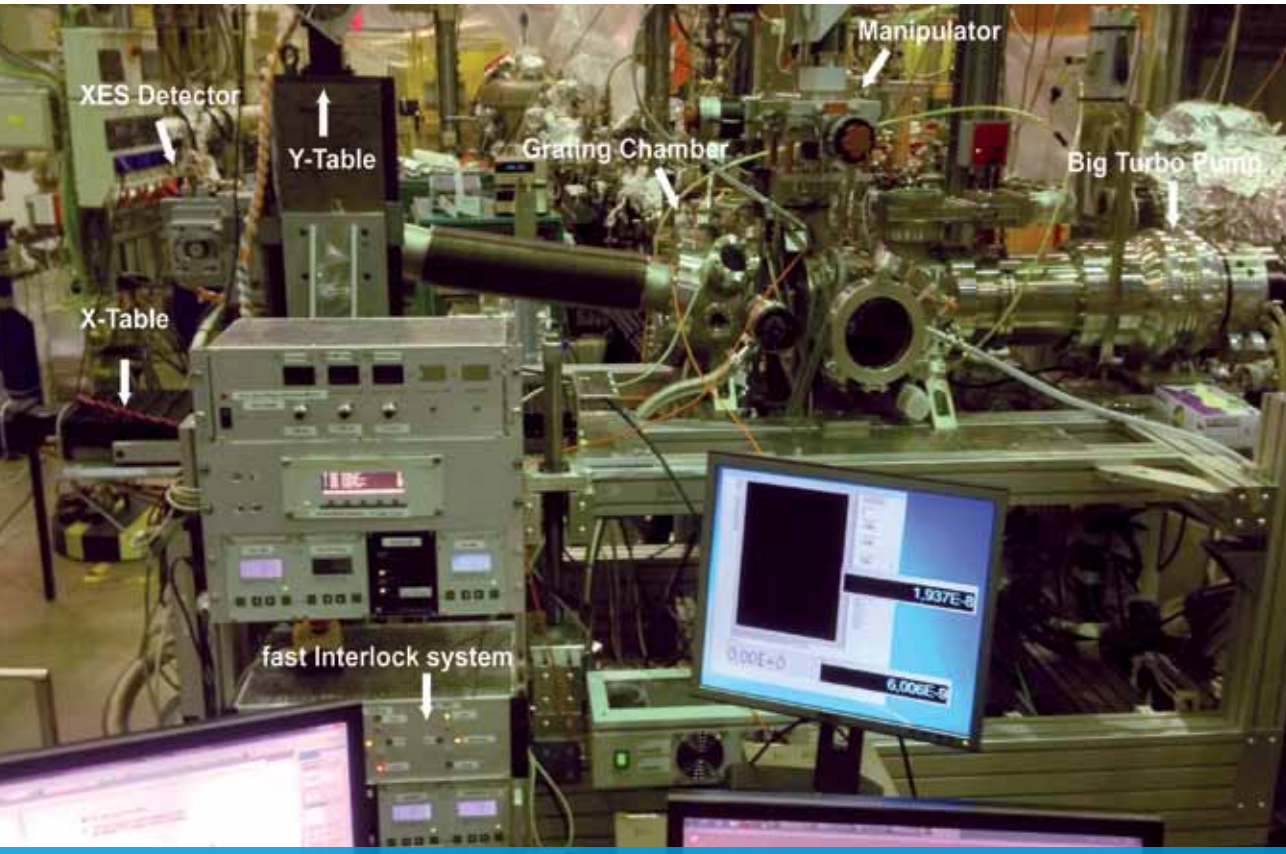

LiXEdrom | XES, XAS, RIXS, Micro-Jet Station

LiXEdrom endstation is equipped with a liquid micro-jet and a soft X-ray emission spectrometer and is dedicated to investigation of functional materials in solution, at surfaces and at interfaces with X-ray absorption (XAS) and resonant inelastic X-ray scattering (RIXS) techniques.

The liquid solution is pumped into the experimental chamber through a circular glass capillary of 15 - 25 µm diameters at a flow rate of 0.35 - 1.5 ml/min and flow speed of around 40 m/s. The continuous freshly introduced solution enables X-ray experiments free of radiation damage which is a crucial prerequisite in investigation of soft matter and biological systems. To preserve the ultra-high vacuum conditions required for soft X-ray experiments the LiXEdrom station is equipped with multi-stage pumping, liquid nitrogen cryo-traps and pinholes that reduce the effective pressure by several orders of magnitude. Operating pressure in the main chamber is $1\text{-}3 \cdot 10^{-5}$ mbar, in the detector chamber is $1 \cdot 10^{-8}$, while at the connection to the beamline the pressure is $5 \cdot 10^{-9}$ mbar.

The X-ray spectrometer operates at grazing incidence angle and Rowland circle geometry. It is equipped with four gratings that cover the

whole soft X-ray energy range from 30 eV to 1200 eV. To increase further the energy resolution, the spectrometer is operated at higher (2nd and 3rd) diffraction orders. The detector consists of a stack of micro-channel plates (MCP), a phosphorous screen, and a charge coupled device (CCD). The MCP plates have a very small pore size of 5 µm and a small bias angle in order to increase spatial/energy resolution and detection efficiency at the CCD. They are coated with a thin film of cesium iodide to increase the number of secondary electrons and to enhance the overall detection efficiency. The CCD is from BASLER with an array of 1040 x 1392 pixels and 30 fps.

Instrument data

Monochromator	PGM
Experiment in vacuum	Yes
X-ray spectrometer	Roland Geometry and Grazing Incidence
Scattering geometry	Horizontal, 90° Angle
Energy range	30 – 1200 eV
Detector	CCD coupled to MCP and Fluorescence Screen
Samples	Liquids and Solids
Sample manipulator	High Precision CF63 Manipulator
Micro-jet unit	16 – 25 µm Nozzles
Instrument responsible	Prof. Emad F. Aziz, emad.aziz@helmholtz-berlin.de Dr. Edlira Suljoti, edlira.suljoti@helmholtz-berlin.de

Instrument application

- Investigation of Hydrogen-bond network and Hofmeister effects in aqueous solutions
- Determination of interfacial electronic properties (electron delocalization) at the solute-solvent interface
- Exploring the strength of charge-donation and back-donation at the metal-ligand bond in organometallic and porphyrin complexes
- Observation of electronic structure changes of catalysts in solution and electrolytes along the reaction path
- Investigating the surface chemistry of nanoparticles in solution activated by different surfactants

EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

References / Latest publications

[1] Bokarev, S. I. *et al.*: State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft X-ray Absorption Spectroscopy and Ab Initio Calculations, Physical Review Letters 111 (2013), 083002.

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LiXEdrom- Reference guide for latest publications

PHOENEXS | (Spin Resolved) Photoemission

Built as a system for photoemission and near-edge X-ray absorption, the PHOENEX station is now used for spin- and angle-resolved photoemission exclusively.

The system is built around a modified SPECS Phoibos 150 hemispherical analyzer equipped with a mini Mott polarimeter. The latter has been developed as the first of its kind based on the known trajectories from the Phoibos analyzer. It operates by means of retardation and features two pairs of channeltrons for the two perpendicular spin quantization axes in the sample surface plane for normal emission. For off-normal emission, this axis is correspondingly tilted. An adjustable iris-type aperture allows for an angular resolution down to 1°.

Samples are mounted on a custom built 5 axes manipulator. The system further features two chambers for preparation purposes and a fast entry lock for sample exchange.

Instrument data

Monochromator	Movable station
Experiment in vacuum	Yes
Temperature range	200 K - 300 K
Detector	SPECS Phoibos 150 hemispherical analyser with mini-Mott detector for spin resolution
Manipulators	5 Axes manipulator with two rotational degrees of freedom
Instrument responsible	Dr. Andrei Varykhalov, andrei.varykhalov@helmholtz-berlin.de apl. Prof. Dr. Oliver Rader, rader@helmholtz-berlin.de

Instrument application

- Topological insulators
- Rashba-split surface and quantum-well states
- Exchange interaction systems

Additional techniques and characterization facilities:

- Low energy electron diffraction
- Quadrupole mass spectrometer
- e-Beam evaporators
- Heating stage up to 2000°C
- Ion gun for sample cleaning

References / Latest publications

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[2] Marchenko, D. *et al.*: Spin splitting of Dirac fermions in aligned and rotated graphene on Ir(111). Physical Review B 87 (2013), 115426.

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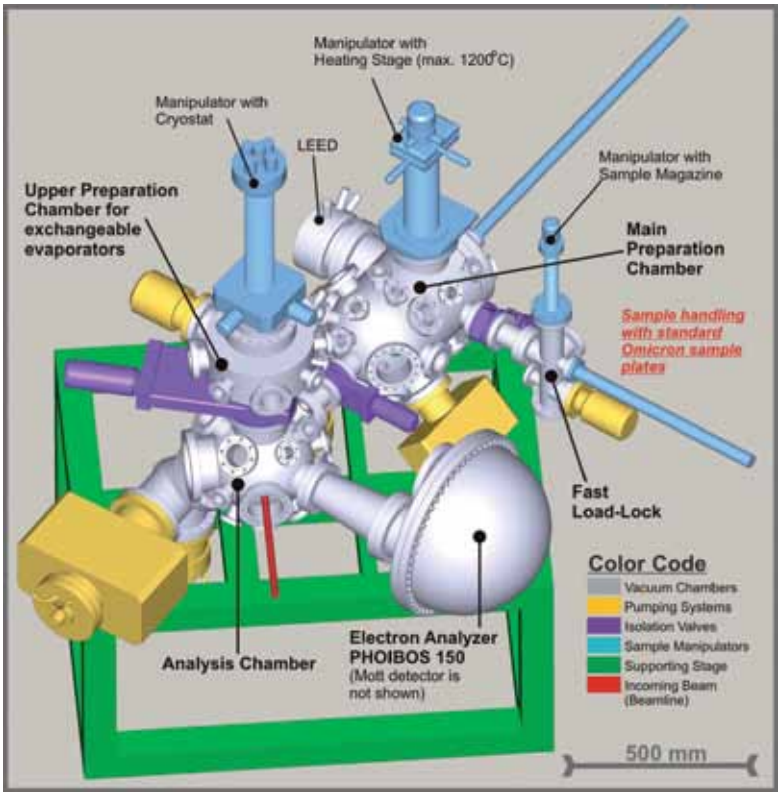


EXPERIMENTAL HALL BESSY II

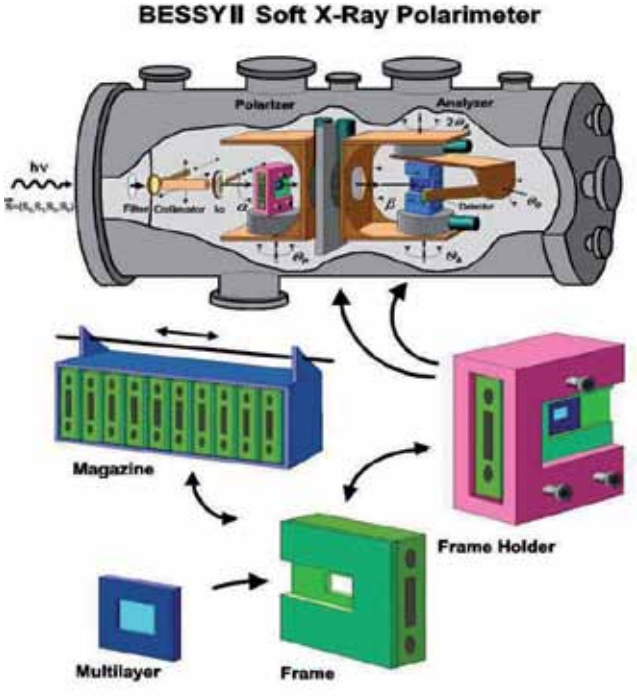
FLEXIBLE STATIONS BESSY II

PHOENEXS - Reference guide for latest publications

Polarimeter | Soft X-ray Polarimeter

The high precision 8-axes ultra-high vacuum compatible (UHV)-polarimeter is a multipurpose instrument which can be used as a selfcalibrating polarisation detector for linearly and circularly polarised UV- and soft X-ray light. It can also be used for the characterisation of either reflection or transmission properties (reflectometer) or polarising and phase retarding properties (ellipsometer) of any optical element. Magneto-optical experiments are possible in transmission, as the XMCD or XMLD (Magnetic Circular / Linear Dichroism) that are intensity measurements.

Additionally a polarisation analysis of the transmitted light is possible which allows for Faraday- or Voigt-measurements. In reflection the magneto-optical Kerr effect can be exploited in longitudinal (L-MOKE) or transversal (T-MOKE) geometry as intensity measurement to investigate thin films as well as magnetic multilayers. Independent two-dimensional rotation of the detector enables any non-specular magnetic scattering experiment on magnetic dots or grains. A load-lock transfer chamber allows for quick and easy sample exchange.



EXPERIMENTAL HALL BESSY II

FIXED STATIONS BESSY II

Instrument data

Experiment in vacuum	10^{-9} mbar
Temperature range	280 - 480 K
Max. sample size	50 x 50 x 11 mm^3
Min. sample size	10 x 10 x 0.5 mm^3
Incidence angle scan range	$0° \leq \Theta_P, \Theta_A \leq 90°$
Azimuthal angle scan range	$0° \leq \alpha, \beta \leq 370°$
Detector scan range (in plane) (off-plane)	$0° \leq \Theta_{2A} \leq 180°$ $-10° \leq \Theta_D \leq 27°$
Min. step size for all motors	0.001°
Sample – Detector Distance	150 mm
Detector	GaAsP-photodiode with Keithley electrometer 617 (6514)
Detector size	4 x 4 mm^2, 0.2 x 4 mm^2
Heating	200 °C
Magazine store	*In-situ* change of 10 samples
Higher order filters	Be, B, C_6H_8, Ti, Cr, Fe
Collimator pinholes	⌀ 0.2 – 2.0 mm
Instrument responsible	Dr. Franz Schäfers, franz.schaefers@helmholtz-berlin.de Dr. Andrey Sokolov, andrey.sokolov@helmholtz-berlin.de

References / Latest publications

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[5] Eriksson, F. *et al.*: Interface Engineering of Short-period Ni/V Multilayer X-ray Mirrors, Thin Solid Films 500 (2006), 84-95.

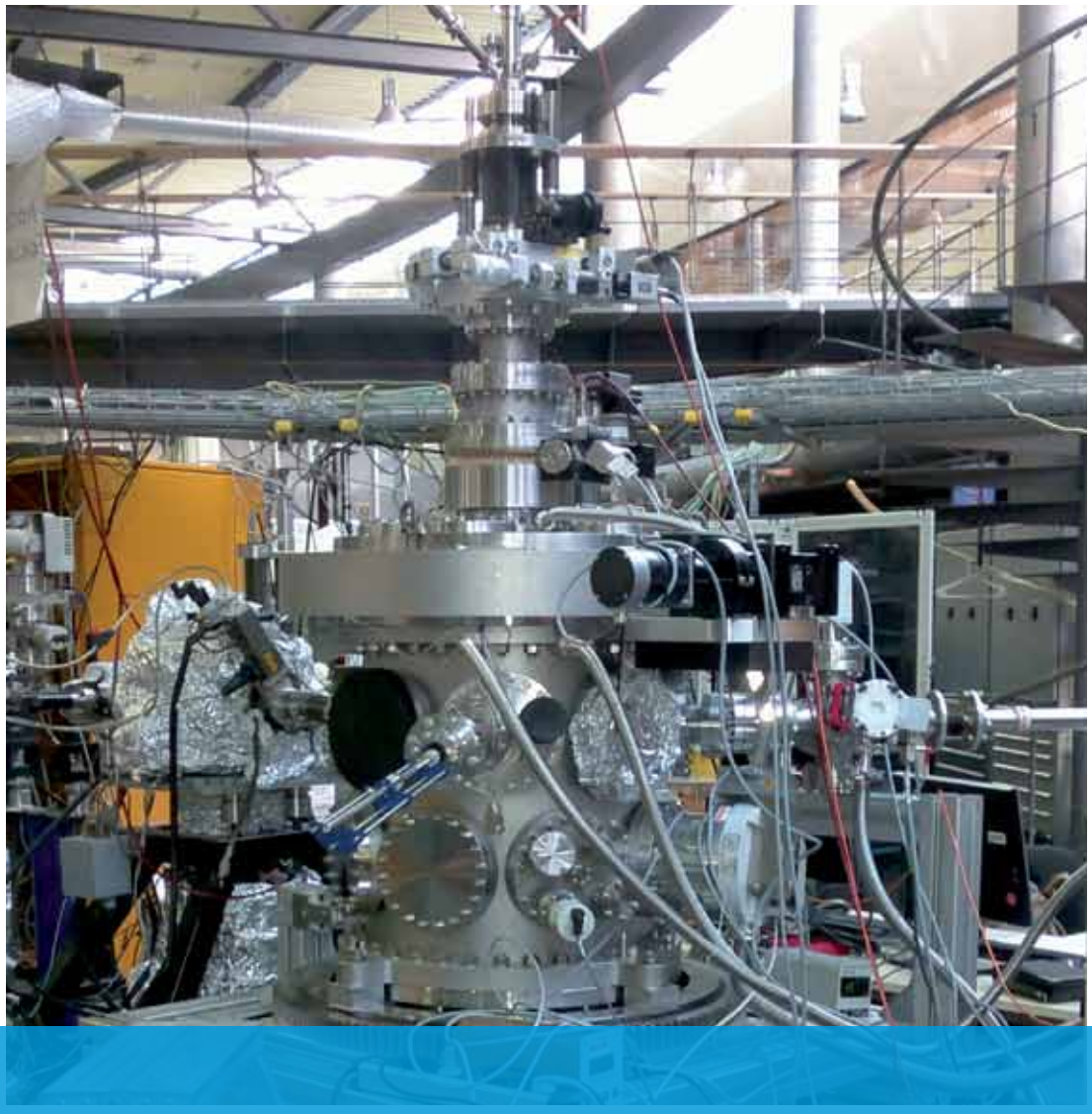
[6] Mertins, H.-Ch. *et al.*: Resonant magnetic reflection coefficients at the Fe 2p edge obtained with linearly and circularly polarized soft x rays, Phys. Rev. B 66 (2002), 184404.

[7] Zaharko, O. *et al.*: Exchange coupling in Fe/NiO/Co film studied by soft X-ray resonant magnetic reflectivity, Phys. Rev. B 66 (2002), 134406.

Instrument application

- Elipsometry, Polarimetry, Reflectometry
- Characterisation of optical elements
- Reflection, transmission properties (s-, p-pol.)
- Polarising properties (phase retardation)
- Determination of polarization of incident light (Stokes S0,1,2,3)
- Resonant Magnetic Scattering (specular and diffuse)
- Intensity spectroscopy: MCD, LMD, Kerr-effect (L, T-MOKE)
- Polarisation spectroscopy: Faraday-, Voigt-effect

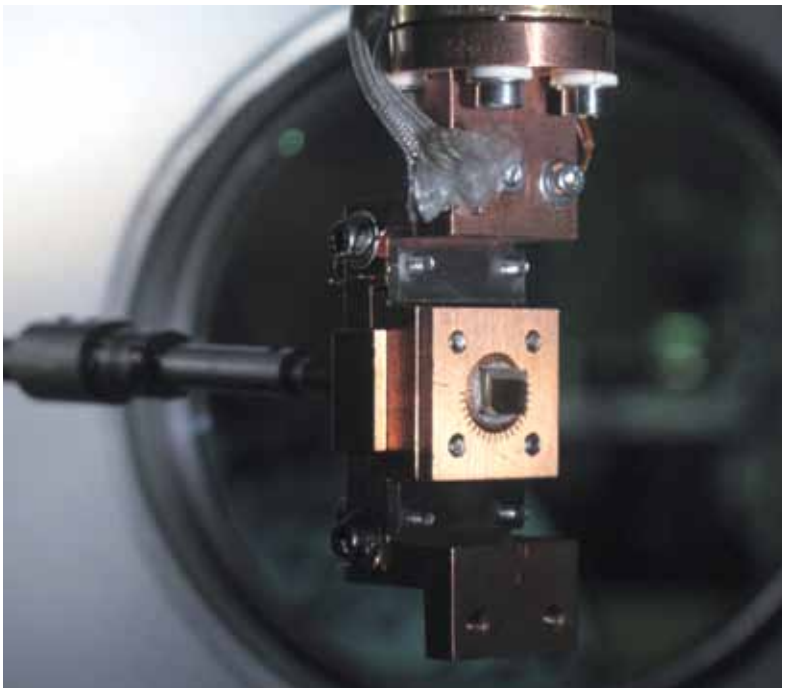
Polarimeter - Reference guide for latest publications



Resonant Scattering | Soft X-ray Scattering

UHV chamber for soft X-ray scattering experiments with in-vacuum CCD detector.

- Different detectors including in vacuum CCD, Si diode, APD detectors can be rotated around the sample.
- Different sample stages for low temperatures (6.5 K ... 300 K) without sample transfer, and either 20 K ... 400 K or 80 K ... 650 K with sample transfer system.
- Motorized x,y,z,th,chi (+- 3 deg) manipulator, manual phi rotation.
- Optional ultra-stable sample stage for XPCS or similar techniques.
- Motorized vertical translation of all detectors.
- Control software SPEC.



EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

Instrument data

Monochromator	Soft X-ray (hard possible)
Experiment in vacuum	Yes
Temperature range	Low-temperature sample holder 6.5 - 300 K, high-temperature sample holder 80 - 650 K
Detector	In-vacuum CCD, photo diode, APD
Manipulators	x, y, z, th, chi, phi (manual)
Instrument responsible	Dr. Christian Schüßler-Langeheine, christian.schuessler@helmholtz-berlin.de Dr. Piter Sybren Miedema, piter.miedema@helmholtz-berlin.de

Instrument application

- Resonant soft X-ray diffraction from nanoscale order in correlated materials
- Magnetic diffraction from antiferromagnetic materials
- Resonant reflectivity from thin films and superstructures
- Domain wall dynamics in magnetic or phase-separated materials
- Absorption spectroscopy

References / Latest publications

[1] Tanaka, A. *et al.*: Analysis of charge and orbital order in Fe_3O_4 by Fe $L_{2,3}$ resonant X-ray diffraction, Phys. Rev. B 88 (2013), 195110.

[2] Beye, M. *et al.*: Stimulated X-ray emission for materials science, Nature 501 (2013), 191.

[3] Huijben, M. *et al.*: Defect Engineering in Oxide Heterostructures by Enhanced Oxygen Surface Exchange, Advanced Functional Materials 23 (2013), 5240.

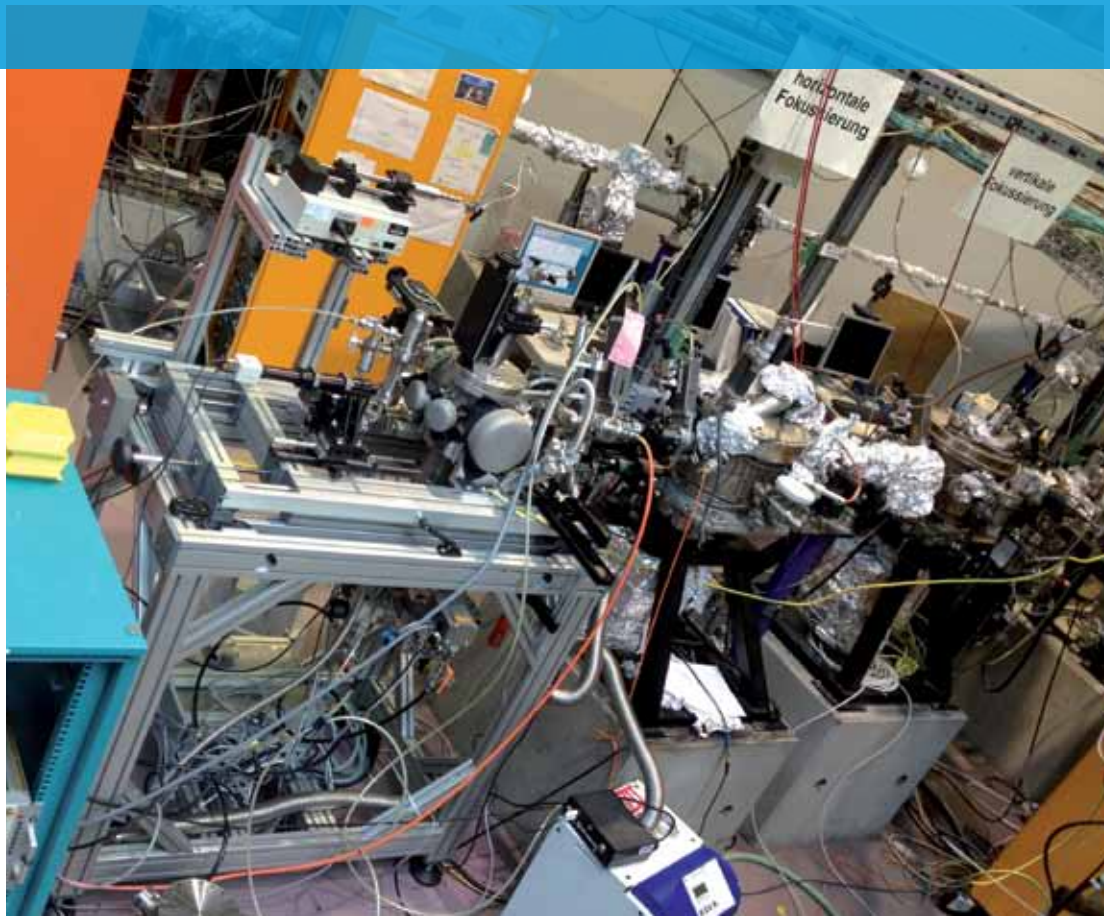
Resonant Scattering - Reference guide for latest publications

Transmission NEXAFS | Time-resolved and steady-state soft X-ray absorption spectroscopy on liquid samples

This is an end station for time-resolved and steady-state soft X-ray absorption spectroscopy (XAS/NEXAFS/XANES/EXAFS) in transmission on liquid samples. The liquid is held between two SiN membranes in He (several 10 mbar) and forms a thin film. The film thickness can be varied between 50 nm and several µm.

It has been demonstrated that saturation effects which tend to dominate fluorescence yield modes of measuring X-ray absorption spectra can be avoided in the transmission cell, permitting a truer capturing of a sample's absorption cross-section.

The Transmission NEXAFS endstation has been used to investigate the O-K edge NEXAFS of liquid water. It has also measured O-K and metal-L edge NEXAFS of aqueous solutions of 3d metal ions. It is possible to heat the solutions and perform temperature dependent NEXAFS using a modified sample holder.



Instrument data

Monochromator	Flexible (soft X-rays)
Experiment in vacuum	Yes
Temperature range	Room temperature
Detector	GaAsP diode or APD
Samples	Thin liquid films
Instrument responsible	Dr. Wilson Quevedo, wilson.quevedo@helmholtz-berlin.de Priv.-Doz. Dr. Philippe Wernet, wernet@helmholtz-berlin.de Dr. Brian O' Cinneide, brian.ocinneide@helmholtz-berlin.de

References / Latest publications

[1] Schreck, S. *et al.*: A sample holder for soft X-ray absorption spectroscopy of liquids in transmission mode, Rev. Sci. Instrum. 82 (2011), 103101.

[2] Kunnus, K. *et al.*: From Ligand Fields to Molecular Orbitals: Probing the Local Valence Electronic Structure of Ni^{2+} in Aqueous Solution with Resonant Inelastic X-ray Scattering, J. Phys. Chem. B 117 (2013), 16512.

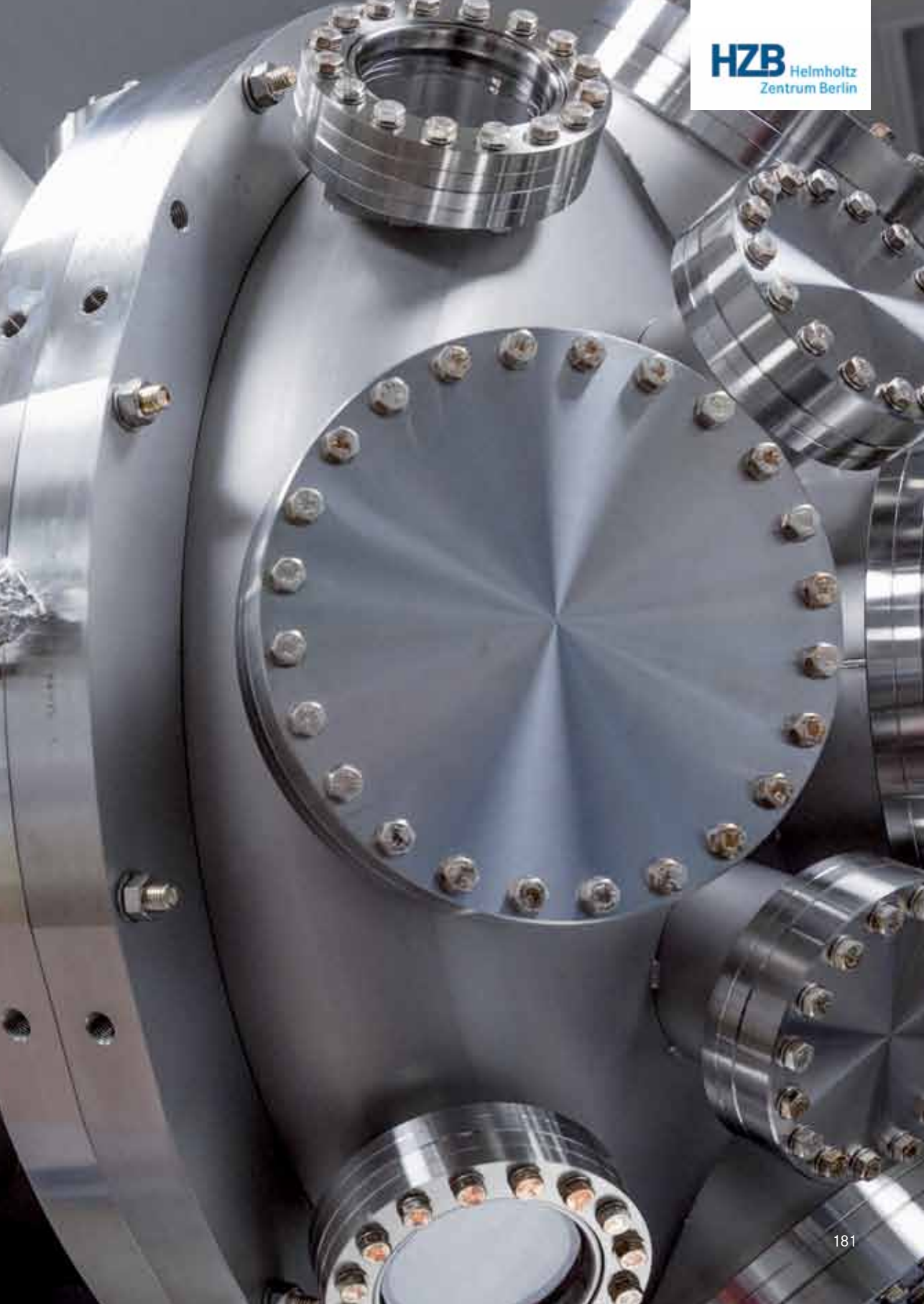
EXPERIMENTAL HALL BESSY II

FLEXIBLE STATIONS BESSY II

Transmission NEXAFS - Reference guide for latest publications

BESSY II

Projects


HZB
Helmholtz
Zentrum Berlin

EMIL | Energy Materials *In-Situ* Laboratory Berlin

The Helmholtz-Zentrum Berlin is currently constructing EMIL, the Energy Materials *In-situ* Laboratory. EMIL is a state of the art laboratory for the preparation and analysis of energy materials. By combining cutting edge, interdisciplinary research with industrially related technologies EMIL seeks to develop new materials and device concepts for solar energy and catalysis research. This unique infrastructure for energy research is a joint project between the HZB and the Max-Planck-Gesellschaft.

The building for EMIL will be finished at the end of 2014 and connected directly to the BESSY II storage ring. The building will initially house two laboratories. SISSY (Solar Energy Materials In-situ Spectroscopy at the Synchrotron) will focus on photovoltaic material and device research and be operated by the HZB. The Fritz Haber Institute of the Max Planck Society will operate the CAT laboratory (Catalysis Research for a Sustainable Energy Supply) where scientists will investigate catalytic and photocatalytic processes.

Instrument application

EMIL's research will address some of modern society's most pressing issues. The sun will play a central role for sustainable energy generation with renewable sources. To deliver the required amount of energy worldwide, however, the cost of solar energy must be reduced. The scientists working in EMIL will explore materials for more efficient photovoltaic cells and new catalytic processes for future solar energy generation and storage concepts. They will develop, analyze and characterize these materials with basic energy research methods but prepare them with industrially related methods. The ultimate goal of the scientists at EMIL is rapid industrial implementation of their research findings.

PROJECTS

- Thin-film silicon systems
- Compound semiconductor materials
- Organic photovoltaic materials
- Micro- and nano-structured PV materials
- Photocatalysts

Contact: Prof. Dr. Klaus Lips,
lips@helmholtz-berlin.de

EMIL - Reference guide for latest publications

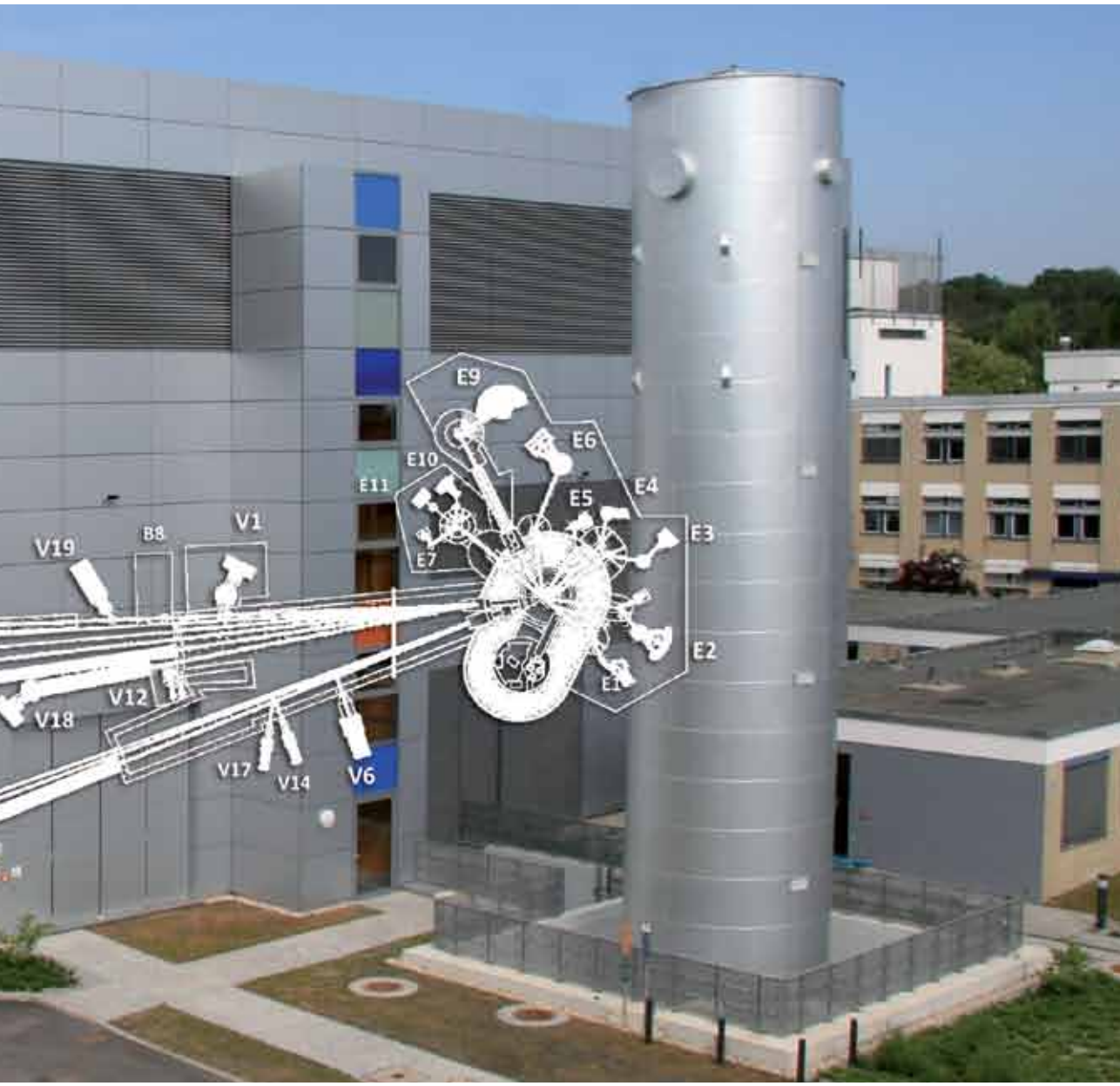
HZB Neutrons at BER II

EXPERIMENTAL HALL BER II

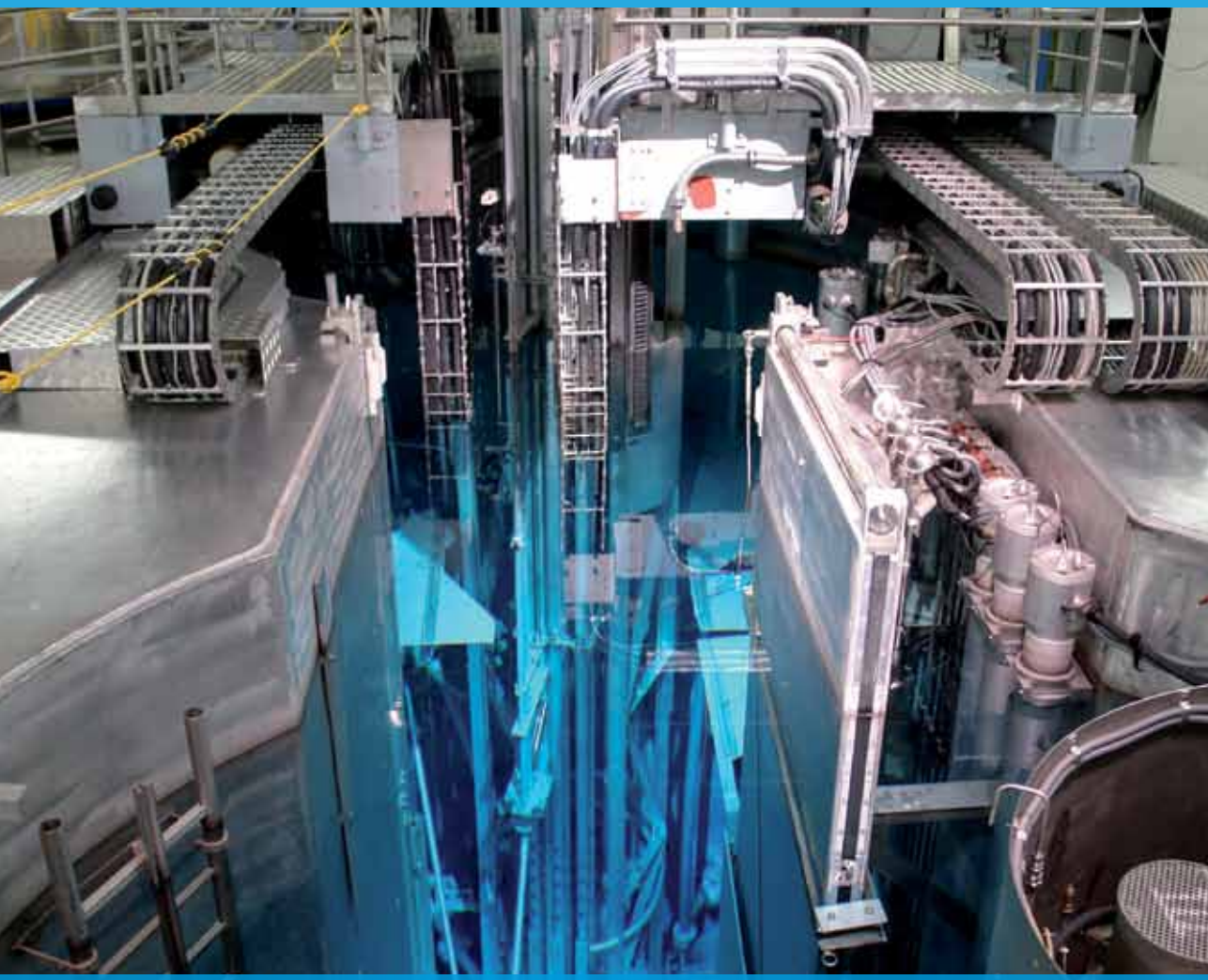
NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

INSTRUMENTS CRG BER II



Neutron source BER II



The neutron facility BER II operated by the Helmholtz-Zentrum Berlin is one of the two German facilities for neutron scattering research and one of the best and most widely used neutron sources in Europe. BER II is open to the international community of all kinds of disciplines. It offers access to a great variety of new or upgraded neutron scattering instruments, suited for research in many fields of science. A large range of sample environment equipment is available to carry out experiments under extreme sample conditions.

The research reactor BER II at the Helmholtz-Zentrum Berlin is a light water cooled and moderated swimming pool type reactor to be operated at 10 MW thermal power. Fuel and control elements are MTR type mounted on a grid plate with 42 positions. The BER II was converted from HEU (High Enriched Uranium)

to LEU (Low Enriched Uranium) core and is now in operation with LEU-core since January 2000. The core configuration operates with 24 fuel elements and uses six additional control elements. The remaining grid positions are filled with reflector elements and irradiation tubes. The core is surrounded by a beryllium reflector wherefrom nine cylindrical beam tubes deliver thermal neutrons to the experiment hall. In addition there is a conical beam tube with a horizontally inserted cold source. The cold source is operated at temperatures of 25-35 K with hypercritical hydrogen in the pressure range of 14-17 bar.

Eight neutron guides deliver cold neutrons from the cold moderator cell to two neutron guide hall adjacent to the experiment hall. Since 2005 a multi-spectral beam extraction guide (NL4a) faces both moderators and supplies the EXED instrument with a wide spectrum of cold and thermal neutrons.

The undisturbed thermal neutron flux density in the beryllium reflector amounts to $1.2 \cdot 10^{14}$ n/cm^{2}s. The disturbed thermal neutron flux density was measured at $7 \cdot 10^{13}$ n/cm^{2}s in a tangential beam tube and $8.6 \cdot 10^{13}$ n/cm^{2}s in a radial beam tube. The capture flux density was measured at the end of a ^{58}Ni coated neutron guide at $1.1 \cdot 10^{9}$ n/cm^{2}s.

A view on the instruments and the sample environment available at BER II at HZB is given in this brochure. HZB puts special emphasis on providing expert support to scientists with no previous experience in neutron scattering and on service for the special needs of young scientists and students.

Neutron source specifications

- **Year:** construction finished 1972, operation started 1973
- **Upgrade I:** 1985 upgrade to10 MW, installation of cold source, reopening 1991
- **Type:** open, light water moderated swimming pool reactor
- **Pool measurements:** 200 m³ water capacity, two pools each 3.5 m in diameter and 11 m deep linked by a channel 2 m wide
- **Delivery:** - 10 MW of thermal power
  - about 2 x 10^{14} neutrons per square cen timetre and second in the core
- **Fuel elements:** conversion to low enriched uranium 1998-2000, 24 standard elements each with 322 g of U-235 and 6 elements for receiving the control rods each with 238 g of U-235
- **Control rods:** 6 neutron absorbers
- **Reflector:** 32 cm beryllium jacket
- **Beam holes:** 9 beam holes (experimental hall)
- **Neutron guides:** 9 neutron guides
- **Upgrade II:** new in-pile part, new cold source / moderator cell, refurbished neutron guides

BER II

Instruments E-Hall

HZB Helmholtz Zentrum Berlin

E2 | Flat-Cone Diffractometer

A 3-dimensional part of the reciprocal space can be scanned in less than five steps by combining the “off-plane Bragg-scattering” and the flat-cone layer concept while using a new computer-controlled tilting axis of the detector bank. Parasitic scattering from cryostat or furnace walls is reduced by an oscillating „radial“ collimator. The datasets and all connected information is stored in one independent NeXus file format for each measurement and can be easily archived. The software package TVneXus deals with the raw data sets, the transformed physical spaces and the usual data analysis tools (*e.g.* MatLab). TVneXus can convert to various data sets *e.g.* into powder diffractograms, linear detector projections, rotation crystal pictures or the 2D/3D reciprocal space.

For single crystal work the multi detector bank (four 2D detectors 300x300 mm^2) and the sample table can be tilted around an axis perpendicular to the monochromatic beam to investigate upper layers in reciprocal space (Flat-Cone technique). For powder studies, the multi detector bank set on only two positions for a measure the a powder diffractogram of 80° or every detector can be set on an individual position (with gaps between the detectors) for *in-situ* measurements.

EXPERIMENTAL HALL BER II

INSTRUMENTS BER II

Instrument application

- Complicated distributions of Bragg and superstructure reflections in three dimensions of reciprocal space (Flat-Cone)
- Low intensity sublattice scattering patterns
- Diffuse scattering arising from structural and magnetic disorder
- Magnetic and crystal structures
- *In-situ* kinetic of phase transitions and chemical reations

Selected examples

- Dirac Strings and Magnetic Monopoles in the Spin Ice $D_{y\text{-}2}Ti_2O_7$, Morris *et al.*, Science 326 (5951): 411-414 (2009)
- Patterning of sodium ions and the control of electrons in sodium cobaltate, M.Roger et. al, Nature 445, 631-634 (8 February 2007)
- Magnetic phase control by an electric field, Th. Lottermoser *et al.*, Nature 430, 541-544 (29 July 2004)
- Electronic Structure and Nesting-Driven Enhancement of the RKKY Interaction at the Magnetic Ordering Propagation Vector in Gd_2PdSi_3 and Tb_2PdSi_3, D. Isonov et al., Phys. Rev. Lett. 102, 046401 (2009)
- Magnetic interaction parameters from paramagnetic diffuse neutron scattering in MnO, D. Hohlwein *et al.*, Phys. Rev. B 68, 140408(R) (2003)

The detector shielding is optimized for the best signal-to-background ratio.

HZB Helmholtz Zentrum Berlin

References / Latest publications

[1] Levy, D. *et al.*: Structure of magnetite (Fe_3O_4) above the Curie temperature: a cation ordering study, Physics and Chemistry of Minerals 39 (2012), 169-176.

[2] Meier, D. *et al.*: Mutual induction of magnetic 3d and 4f order in multiferroic hexagonal $ErMnO_3$, Physical Review B 86 (2012), 184415.

[3] Rolfs, K. *et al.*: Key Properties of Ni-Mn-Ga Based Single Crystals Grown with the SLARE Technique, Advanced Engineering Materials 14 (2012), 614-635.

[4] Morris, D. *et al.*: Dirac Strings and Magnetic Monopoles in the Spin Ice $Dy_2Ti_2O_7$, Science 326 (2009), 411-414.

[5] Roger, M. *et al.*: Patterning of sodium ions and the control of electrons in sodium cobaltate, Nature 445, 631-634 (8 February 2007)

[6] Lottermoser, Th. *et al.*: Magnetic phase control by an electric field, Nature 430 (2004), 541-544.

[7] Isonov, D. *et al.*: Electronic Structure and Nesting-Driven Enhancement of the RKKY Interaction at the Magnetic Ordering Propagation Vector in Gd_2PdSi_3 and Tb_2PdSi_3, Phys. Rev. Lett. 102 (2009), 046401.

[8] Hohlwein, D. *et al.*: Magnetic interaction parameters from paramagnetic diffuse neutron scattering in MnO, Phys. Rev. B 68 (2003), 140408(R).

Instrument data

Beam tube	R 1B
Collimation	15‘, 30‘, 60‘ (open)
Monochromator	• Cu (220) • Ge (311) • PG (002)
Wave length	• λ=0.091 nm [Cu (200)] • λ=0.121 nm [Ge (311)] • λ=0.241 nm [PG (002)]
Flux	$2 \cdot 10^6$ n/cm^{2}s (flat PG monochromator without collimation)
Range of scattering angles	-10°< 2 Θ< 107°
Angle resolution	• Horizontal resolution: 0.2° - 0.1° • Vertical resolution: 0.5° - 0.1° • Pixel size 0.1°x0.1°
Detector	Four 2D delay-line detectors (PSD 300 x 300 mm^2)
Polarized neutrons	No
Instrument options	• Single crystal mode • Powder diffraction mode
Software	TVneXus
Tilting angle	0°< μ < 18°
Instrument responsible	Dr. Jens-Uwe Hoffmann, hoffmann-j@helmholtz-berlin.de Dr. Illia Glavatskyi, illya.glavatskyy@helmholtz-berlin.de

E2 - Reference guide for latest publications

E3 | Residual Stress Analysis and Texture Diffractometer

The diffractometer is designed for strain and stress analysis for simple geometric samples as well as for industrial applications and heavy components of arbitrary shape. The diffractometer itself consists of two big omega circles (Ω and 2Θ) with a diameter of 800 mm and upon a translation table (xyz-direction) for sample positioning in vertical and horizontal direction. This set up is installed for handling heavy and/or large samples and components such as impellers or turbines with diameters of up to half a meter and loads up to 300 kg. A range of equipment for sample positioning is available, such as a closed Eulerian cradle for samples with weights of up to 5 kg. A second cradle for heavy samples (up to 50 kg) with the ability to tilt the samples up to 90° is used to measure three perpendicular sample orientations. Gauge volumes can be adjusted horizontally and vertically by a computer-controlled variable primary slit in a range from 0-10 mm and 0-20 mm respectively. Rapid data visualization as well as evaluation is performed by the specially designed software SteCa.

The recent upgrade activities have significantly increased the range of applications on E3:

- Monochromator upgrade (2007): A set of perfectly bent Si (400) crystals providing a neutron wavelength of 0.1486 nm focusses on the sample. Thus the E3 has become faster and more adaptable to different types of measurement.
- Electronics upgrade (2011): New motor control system and detector electronics have been implemented providing a reliable and modular interface between instrument and the CARESS control software.
- Radial collimator (2012): An oscillating collimator secondary optic has been implemented to improve the instrument resolution, especially at interfaces.
- New Eulerian cradle and stress rig (2013): An open tilt stage to measure three perpendicular strain directions within one sample alignment has been installed. The same is possible with a new custom-developed stress rig for tension and compression experiments with loads of up to 50 kN.
- New motorized primary slit (2013): E3 is now equipped with a primary slit device to change the gauge volume without instrument re-calibration (in both vertical and horizontal directions).
- Laser scanner (2014): A new laser scanner system is to be implemented on E3 to make instrument (re-)calibration and sample alignment much faster and more precise.

Instrument data

Beam tube	T 2
Collimation	Open
Monochromator	Si (400), double focussing
Take off angle of monochromator	65°
Wave length	0.1486 nm
Flux	~ 10^7 n/cm^2/s
Range of scattering angles	35° ≤ 2Θ ≤ 110°
FWHM standard powder	~ 0.3 (at 2Θ= 90°)
Detector	Position-sensitive area detector 30 x 30 cm^2
Resolution	$\Delta d/d \approx 1.4 \cdot 10^{-3}$
Sample to detector distance	600 to 1300 mm
Beam size at sample	max: 10 x 20 mm^2
Maximum sample size	0.5 m diameter
Scan range	• 200 mm (sample position scans) • ~ 35° ≤ 2Θ ≤ 110° (peak position scans)
Polarized neutrons	No
Instrument options	• Texture option • Variable slit systems • Radial collimator
Sample environment	• x-y-z table for max. 300 kg • Eulerian cradles • Stress rigs (tension, compression, torsion)
Software	SteCa, TVtueb (analysis), CARESS (instrument control)
Instrument responsible	Dr. Robert Wimpory, robert.wimpory@helmholtz-berlin.de Dr. Mirko Boin, boin@helmholtz-berlin.de

Instrument application

- Residual stress analysis on monocrystalline or polycrystalline materials and machine components
- *In-situ* residual stress analysis within industrial components during mechanical (up to 50 kN) or thermal loading (up to 2000 K)
- Investigation of local phase transitions
- Texture measurements using Eulerian cradles

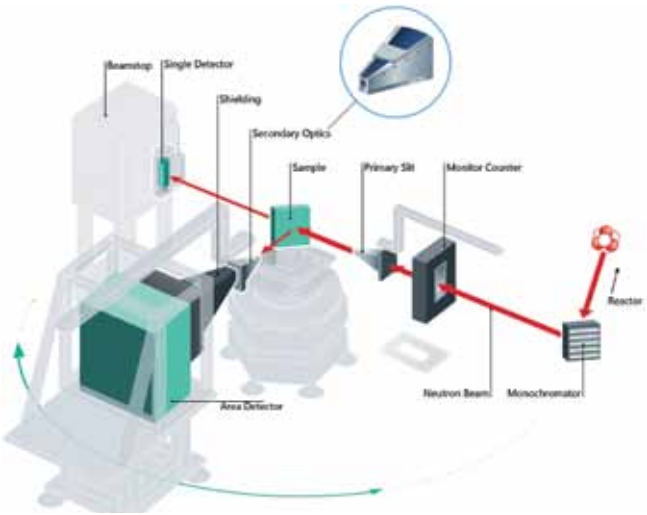
References / Latest publications

[1] Poeste, T. *et al.*: The New and Upgraded Neutron Instruments for Materials Science at HMI - Current Activities in Cooperation with Industry, Mater. Sci. Forum 524-525 (2006), 223-228.

[2] Wimpory, R.C. *et al.*: Efficiency Boost of the Materials Science Diffractometer E3 at BENSC: One Order of Magnitude Due to a Horizontally and Vertically Focusing Monochromator, Neutron News 19 (2008), 16-19.

[3] Requena, G. *et al.*: Neutron Diffraction, InTech (2012), ISBN 978-953-51-0307-3.

[4] Boin, M. & Wimpory, R.C.: Upgrade Activities on the E3 Residual Stress Neutron Diffractometer, Mater. Sci. Forum 768-769 (2014), 31-35.



EXPERIMENTAL HALL BER II

INSTRUMENTS BER II

E3 - Reference guide for latest publications

E4 | Two-Axis Diffractometer

The instrument is primarily suited for magnetic structure determination under various conditions, which includes magnetic fields up to 17 T, temperatures down to 30 mK and hydrostatic pressures up to 10 kbar. The application of uniaxial pressure and use of auxiliary methods (*e.g.* electrical resistivity, ac susceptibility, pyroelectric current measurements) is also possible. The most common application is to reveal spatial arrangement ordered spin structures, to study magnetic and/or crystal structure phase transitions and construction of phase diagrams. Using the polarized neutrons option facilitates the separation of magnetic contributions from nuclear scattering. The measurement of flipping ratios allows registration of very weak magnetic scattering. The monochromator shielding contains three beam channels at 2ΘM = 20°, 42.5° and 65° with the instrument installed at 2ΘM = 42.5° most of the time. This position corresponds to the incident wavelength of 0.244 nm. The additional option of polarized neutrons uses a super mirror bender and a π-flipper. The instrument runs under the system CARESS; automatic control of temperature and magnetic field is provided.

E4 with a Vanadium standard sample on the Irrelec table. On the left is the 2D detector with electronics.

Instrument application

- Magnetic structure determination
- Study of magnetic and structural phase transitions
- Determination of magnetic phase diagrams
- Study of critical points as a function of magnetic field and temperature
- Measurement of correlation functions above the ordering temperature

Instrument data

Beam tube	R 2
Collimation	Automatic change of $\alpha 1$ = 20', 40', open geometrical divergence: $\alpha 1$ = 60', manual variation of $\alpha 2$ (10', 20', 40') and $\alpha 3$ (Soller or oscillating radial)
Monochromator	PG (002) with variable vertical curvature Ge (113) double focusing
Take off angle of monochromator	$2\Theta M$ = 20°, 42.5°, 65°, permanently installed at 42.5°
Wave length	λ=0.244 nm (PG) or 0.122 nm (Ge)
Flux	0.8·106 n/cm^{2}s (PG) 0.6·106 n/cm^{2}s (Ge) 0.3·106 n/cm^{2}s polarized (PG+bender)
Range of scattering angles	0° ≤ 2Θ ≤ 120° (with configurational restrictions related to sample environment)
Angle resolution	Depends on setting
Sample size	From 1mm^3 for topic-focused studies
Detector	2D detector 200x200 mm^2 (removable oscillating radial collimator in front), variable distance (640-900 mm)
Polarized neutrons	Yes (super mirror bender) Please contact the instrument scientist to discuss in advance
Instrument options	Polarization analysis (super mirror analysis)
Sample environment	• Horizontal magnetic field < 6 T • Vertical magnetic field < 17 T • Temperature range 0.03 - 600 K • Hydrostatic pressure 0 - 10 kbar • 4-circle mode
Software	CARESS, BEAN, set of supporting programs to deal with 2D data
Instrument responsible	Dr. Karel Prokes, prokes@helmholtz-berlin.de Dr. Vadim Sikolenko, vadim.sikolenko@helmholtz-berlin.de

References / Latest publications

[1] Piatek, J.O. *et al.*: Phase diagram with an enhanced spin-glass region of the mixed Ising-XY magnet $LiHo_xEr_{1-x}F_4$, Physical Review B 88 (2013), 014408.

[2] Tsyrulin, N. *et al.*: Ressouche, E.; Paduan-Filho, A.; Kenzelmann, M.: Neutron study of the magnetism in $NiCl_2{\cdot}4SC(NH_2)_2$, Journal of Physics: Condensed Matter 25 (2013), 216008.

[3] Artyukhin, S. *et al.*: Solitonic lattice and Yukawa forces in the rare-earth orthoferrite $TbFeO_3$, Nature Materials 11 (2012), 694.

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[5] Liu, T.J. *et al.*: From (0,π) magnetic order to superconductivity with (π,π) magnetic resonance in $Fe_{1.02}Te_{1-x}Se_x$, Nature Materials 9 (2010), 716.

EXPERIMENTAL HALL BER II

INSTRUMENTS BER II

E4 - Reference guide for latest publications

E9 | Fine Resolution Powder Diffractometer (FIREPOD)

The Fine Resolution Powder Diffractometer E9 (FIREPOD) is an angle-dispersive powder diffractometer optimized for a flat resolution function with a minimum width of the reflections at the 2Θ-region with the highest density of reflections. The monochromator is placed at a distance of 11 m from the reactor core, which allows for a large take-off angle at the monochromator. An evacuated beam tube and a sapphire single crystal filter reduce air scattering and epithermal neutrons. Neutron flux at the sample is increased by an adjustable vertically focusing Ge-monochromator. The detector consists of eight individual DENEX ^{3}He 2D detectors with 300 x 300 mm active area each and a common radial collimator to reduce background noise. The individual detectors are arranged in a novel setup, at optimized, non-constant distances from the sample. Five of the individual detectors can be placed close to the sample in a high intensity conformation. Data collection with fixed detector position measures parts of the 2Θ-range with increased intensity and without loss in quality. Position-sensitive data integration of the Debye cones results in a strongly reduced asymmetry of the peaks. The 2D-data are directly accessible, allowing the early detection of preferred orientation or spottiness. Depending on sample scattering power and volume and the resolution settings of the instrument, full powder diffraction patterns of a quality suitable for Rietveld refinement can be collected as fast as 30 minutes. With small 1 cm^3 samples and high resolution, between 1 and 6 hours should be estimated, depending on the scattering power of the sample. Scans measuring only a selected angular with fixed detector position can be as fast as 10 minutes per step for good scatterers.

Instrument data

Beam tube	T5
Collimation	α_1: 10' or 18' α_2: 20'
Monochromator	Axially focusing, Risø design, 300 mm height 19 Germanium composite plates with reflecting planes (311), (511), and (711) (511) normal to crystal surface Mosaicity FWHM = 17´
Take off angle of monochromator	50° ≤ 2Θ ≤ 130° 111.7(1)° is used by default
Wave length	λ = 1.3084(2) Å from Ge(711) λ = 1.7982(1) Å from Ge(511) λ = 2.8172(2) Å from Ge(311) & PG filter
Flux	≈ 10^5 n/cm^2s
Range of scattering angles	3° < 2Θ < 142°
Angle resolution	0.33°
Range of lattice spacing	25 Å < d < 0.7 Å from Ge(711) 35 Å < d < 1.0 Å from Ge(511) 55 Å < d < 1.5 Å from Ge(311)
d resolution	≈ $2 \cdot 10^{-3}$
Sample size	1 cm^3 - 5 cm^3
Detector	Eight area detectors (300 mm x 300 mm) Oscillating radial collimator for background reduction
Polarized neutrons	No
Instrument options	Variable sample – detector distance for five of the individual area detectors
Sample environment	OS, OF, HTF, VM3, VM5, DEGAS
Software	CARESS, BEAN
Instrument responsible	Dr. Alexandra Franz, alexandra.franz@helmholtz-berlin.de Dr. Michael Tovar, tovar@helmholtz-berlin.de Dr. Andreas Hoser, hoser@helmholtz-berlin.de

Instrument application

- Crystal structure determination
- Rietveld refinement
- Site occupation factors, *e.g.* of isoelectronic elements
- Determination of light atoms (*e.g.* H, Li)
- Rapid parameterized scans of selected angular regions of the diffraction pattern, *e.g.* temperature or magnetic field strength
- Non-destructive bulk phase analysis

EXPERIMENTAL HALL BER II

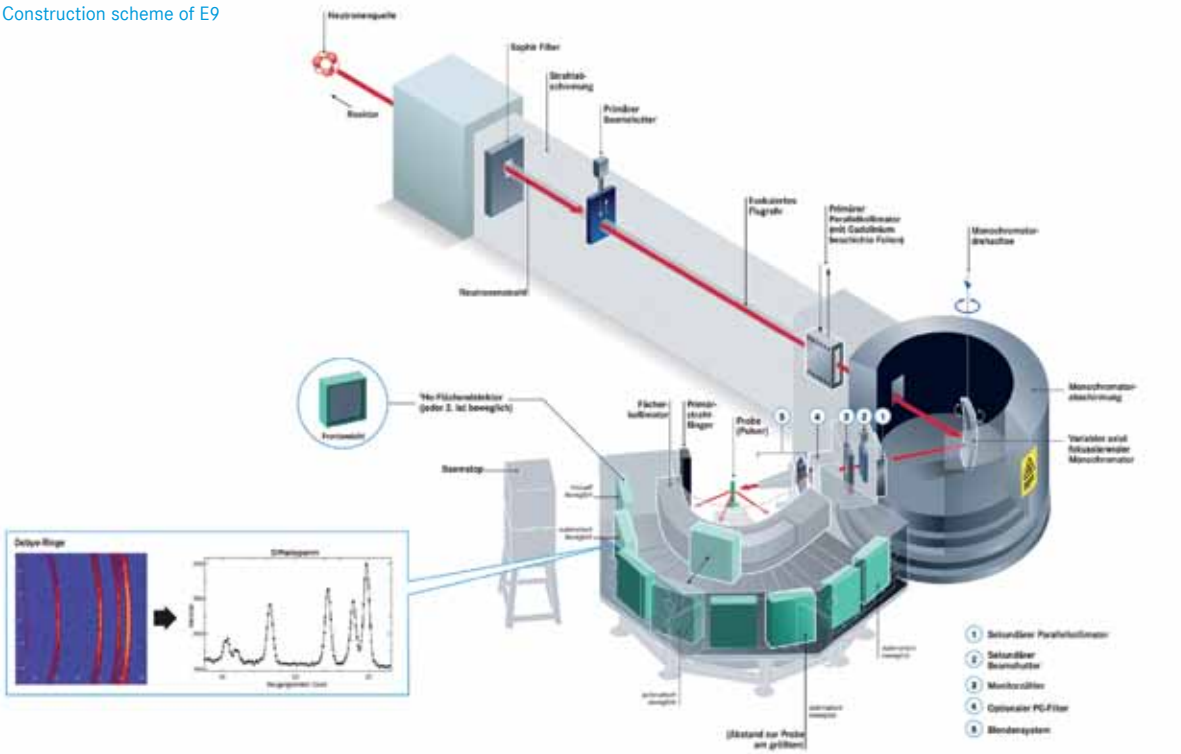
INSTRUMENTS BER II

-> please continue on the next page

E9 - Reference guide for latest publications

E9 | continued

Construction scheme of E9



References / Latest publications

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[2] Paul, A.K. *et al.*: Lattice instability and competing spin structures in the double perovskite insulator Sr_2FeOsO_6, Physical Review Letters 111 (2013), 167205.

[3] Stephan, C. *et al.*: Cationic point defects in $CuGaSe_2$ from a structural perspective. Applied Physics Letters 101 (2012), 101907.

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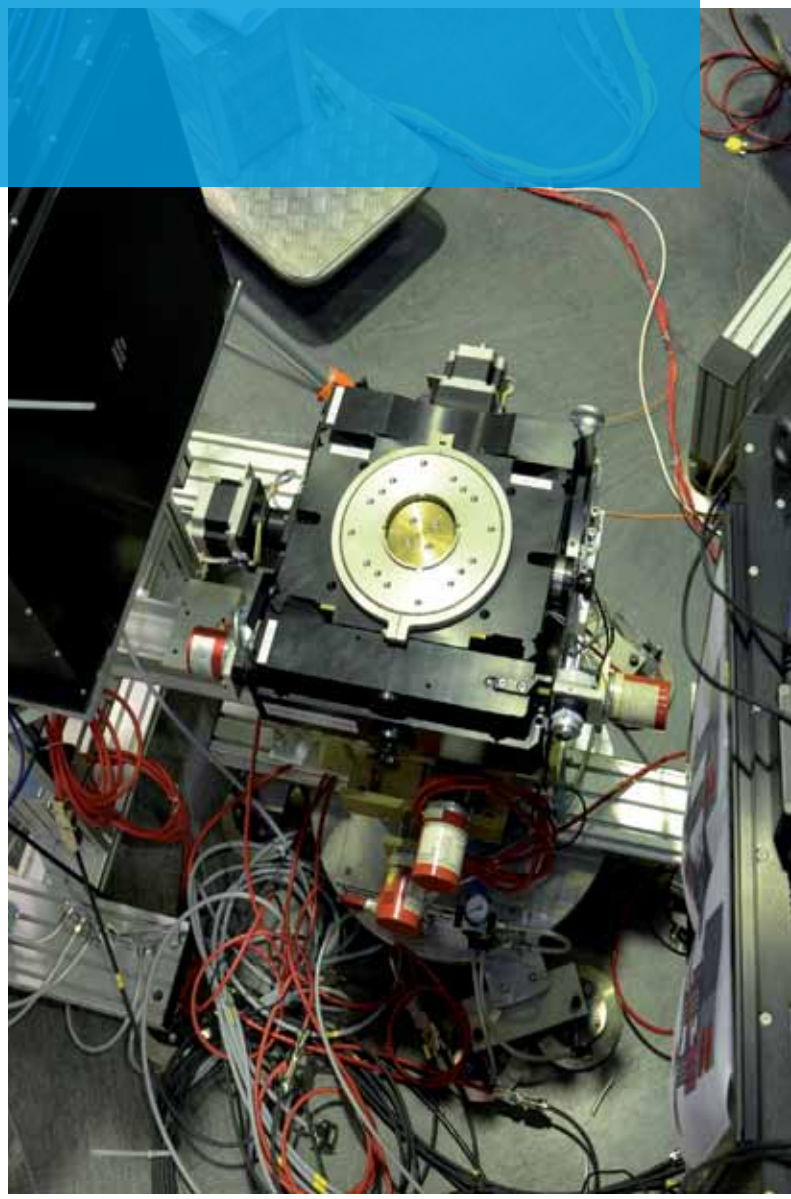
E11 | Fast Acquisition Laue Camera for Neutrons (FALCON)

Neutron Laue diffraction is an important method of neutron scattering for measuring single crystals. Laue diffraction patterns are generated in a matter of seconds from very small crystals i.e. <1 mm^3. FALCON has two scintillating plate detectors coupled to four iCCD cameras each, to produce a 2D projection of a large volume of reciprocal space in a single Laue pattern. Such images can be used to index complex crystal structures, characterize features such as twinning or preferred orientation whilst phase transitions can be investigated using a full range of sample environments including Low/High temperature, Magnetic field and High Pressure and combinations of these.

Situated at the end of a thermal beamtube in the E-Hall, the instrument uses a 'white' neutron beam *i.e.* range of wavelengths. With no monochromators from other instruments upstream, an unhindered beam of neutrons arrives at the sample.

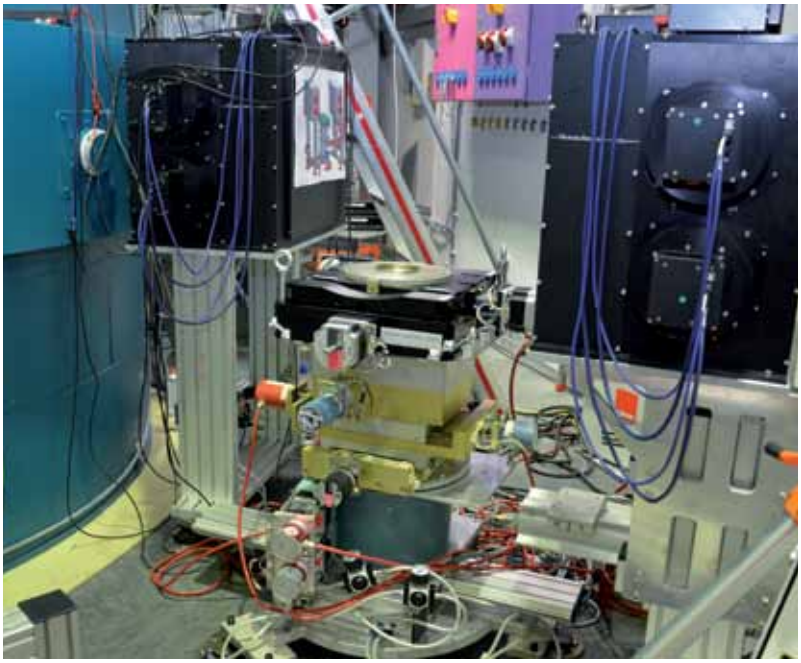


Instrument application

- Point defect analysis in compound semiconductors for energy research
- Complex crystallographic studies *e.g.* twinned crystal structure determination
- *In-situ* kinetics studies
- Low-temperature magnetic studies

Instrument data

Beam tube	D1S
Collimation	Combined shutter/collimator delivering 16 mm diameter beam, with option of additional collimation using 1-10 mm diameter BN noses
Monochromator	N/A
Take off angle of monochromator	N/A
Wave length	$0.8 < \lambda < 5$ Å
Flux	$\approx 10^8$ n cm^{-2} s^{-1}
Range of scattering angles	$3\pi/2$
Sample size	< 1 mm^3
Detector	2x400 mm^2 Li^6 Scintillator plates coupled to 4xiCCD cameras each
Polarized neutrons	No
Instrument options	Ambient: Sample-to-detector distance >10mm Sample Environment: Sample-to-detector distance >160mm
Sample environment	1.5 K < T < 2000 K H < 5 T at 1.5 K < T < 300 K 0 < P < 10 kbar at 1.5 K < T < 600 K
Software	CARESS, MAD
Instrument responsible	Dr. Gail N. Iles, gail.iles@helmholtz-berlin.de



EXPERIMENTAL HALL BER II

INSTRUMENTS BER II

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E11 - Reference guide for latest publications

BER II

Instruments N-Hall

V2 | Cold Neutron 3-Axis Spectrometer (FLEXX)

The instrument name is derived from the flexibility of the spectrometer parameters which permit non-standard experiments and its use in the development of novel methods. The instrument has been recently upgraded and rechristened FLEXX. Its new position at the end of the NL1B guide will allow a larger coverage in wave vector transfer, and the guide itself has been upgraded with m=3 neutron supermirrors to allow more neutrons to be transported from the source to the instrument. In addition, there is an elliptical guide which focuses neutrons onto a virtual source which is subsequently imaged on the monochromator. Finally, a velocity selector is used to select a wavelength band, and so obviate the need for a second order filter and associated loss of neutrons.

With an optimally curved monochromator, the increase in flux at the sample position as compared to the old FLEX is a factor of 5 to 10, at the expense of Q-resolution while retaining the good energy resolution of a cold TAS.

The flexibility of the instrument comes from the ability to choose the distances between the monochromator and sample, between the sample and analyzer and between the analyzer and detector in order to obtain an optimal scattering geometry at the required angular and energy resolutions. For the same purpose a tunable curved (double focusing) monochromator and (horizontally focusing) analyzer are used.

Where possible the spectrometer was made of non-magnetic materials to allow for the use of polarized neutrons in the same set-up as for unpolarized neutrons. For the polarized beam option Helmholtz coils, Mezei flippers and a cavity-type transmission polarizing analyzer may be used, whilst an S-bender polarizer maybe translated into the guide before the elliptical section to minimize neutron losses.

FLEXX provides the opportunity to combine triple axis spectroscopy and high resolution spin-echo spectroscopy. The neutron resonance spin echo method (NRSE) option at FLEXX is particularly suited for the phonon focusing technique with tilted spin echo fields. By this method the line widths of dispersive elementary excitations can be measured with an energy resolution in the μeV range. Before applying for an experiment utilizing the high resolution NRSE option, please contact an instrument responsible directly for a feasibility dialogue.

Instrument application

- Low-energy phonon dispersion
- Soft modes
- Low-energy spin wave dispersion
- Low-energy crystal field exitations
- Quasielastic scattering

with NRSE

- Line widths of low-energy dispersive excitations in non-magnetic and antiferromagnetic samples
- Quasi-elastic linewidths
- High-resolution elastic scattering (Larmor diffraction) with single crystal and powder samples

References / Latest publications

[1] Toft-Petersen, R. *et al.*: High-field magnetic phase transitions and spin excitations in magnetoelectric $LiNiPO_4$, Phys. Rev. B 84 (2011), 054408.

[2] Skoulatos, M. and Habicht, K.: Upgrade of the primary spectrometer of the cold triple-axis spectrometer FLEX at the BER II reactor, Nuc. Instr. Meth. A, 647 (2011), 100.

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[6] Le, M.D. *et al.*: Gains from the upgrade of the cold neutron triple axis spectrometer FLEXX at the BER-II reactor, Nucl. Instr. and Meth. A 729 (2013), 220-226.

NEUTRON GUIDE HALL BER II

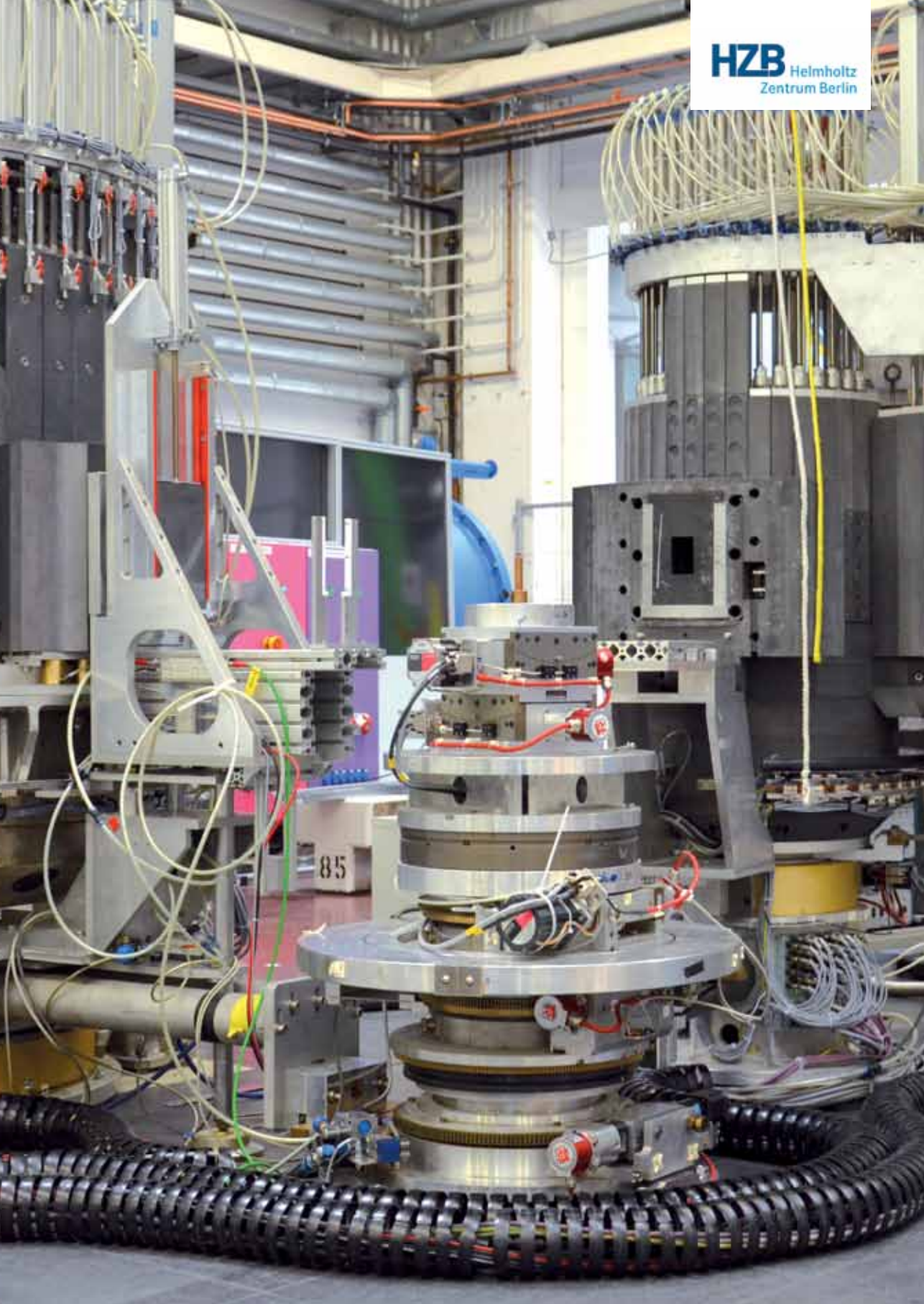
INSTRUMENTS BER II

V2- Reference guide for latest publications

-> please continue on the next page

Instrument data

Neutron guide	NL 1B
Collimation	Gd coated Soller collimators. Before monochromator: 40‘, 60‘ available on a motorised translation table. Before sample, analyzer and detector: 20‘, 40‘, 60‘ available
Monochromator	Pyrolythic graphite (002) with variable vertical and horizontal curvature
Wave length range	2 Å< λ < 6.5 Å
Energy range	1.9 meV < E_M < 27 meV (ΔE range with Φ> $2 \cdot 10^7$ n/cm²s: 0 - 18 meV)
Energy resolution	0.05 to 0.5 meV (FWHM)
Range of scattering angles	-130° < $2\Theta_S$ < 130° (for most configurations)
Detector	Vertical ^{3}He single detector
Analyzer	Pyrolythic graphite (002) with variable horizontal curvature
Range of final energies	2.6 < E_f < 15 meV
Flux	$6 \cdot 10^7$ n/cm²s at 2.5 Å $3 \cdot 10^7$ n/cm²s at 4 Å (with focused monochromator)
ΔE range with Φ>$2 \cdot 10^7$ n/cm²s	0 < ΔE < 18 meV
Filter	Velocity selector and possibility of Be-filter if needed
Polarized neutrons	Yes
Polarizer	Compact S-bender
Instrument options	NRSE option (see specification below)
Sample environment	Can accept all magnet cryostats and dilution sticks at HZB
Software	TASMAD
with NRSE	
Neutron guide	NL 1B
Collimation	Gd coated Soller collimators. Before monochromator: 40‘, 60‘ available on a motorised translation table. Before sample, analyzer and detector: 20‘, 40‘, 60‘ available
Monochromator	Pyrolythic graphite (002) with variable vertical and horizontal curvature
Take off angle of monochromator	67° < $2\Theta_M$ < 150°
Wave length range	0.25 nm < λ < 0.65 nm
Energy range	6 meV < E_M < 27 meV
Energy resolution	In the order of µeV
Range of scattering angles	• Inelastic mode: -110° < $2\Theta_S$ < 110° (with configurational restrictions) • Elastic (Larmor diffraction) mode: -110° < $2\Theta_S$ < 90° or 90° < $2\Theta_S$ < 110°
Detector	Vertical ^{3}He single detector
Analyzer	Heusler
Scattering angle at analyzer	-155° < $2\Theta_A$ < 155°
Flux	$3 \cdot 10^5$ n/cm²s at 0.37 nm
Filter	Velocity selector
Polarized neutrons	Yes
Polarizer	compact S-bender
Instrument options	NRSE option (this specification)
Sample environment	Orange cryostats and closed cycle refrigerators
Software	SEMAD
Instrument responsible	Dr. Diana Quintero Castro, diana.quintero_castro@helmholtz-berlin.de Dr. Rasmus Toft-Petersen, rasmus.toft-petersen@helmholtz-berlin.de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V4 | Small Angle Scattering Instrument (SANS)

V4 allows for the measurement of density composition and magnetization fluctuations in materials on a length scale from 0.5 nm to 400 nm. At short distance the 2D-detector can be moved vertically by 0.17 m, extending the Q range to even higher values. A large sample chamber is connected to the vacuum system with the detector and collimator tubes. Automatic sample changers (both T and B controlled) are available.

A high transmission supermirror polarizer can be introduced by remote control in front of the 12 m collimation without any modification of the instrument alignment. The polarization direction can be reversed by a RF gradient spin-flipper in front of the sample. The SANSPOL option is characterized by a high neutron flux of more than 30% of the non-polarized beam (wavelength dependent), a high degree of polarization (> 90%) and high efficiency of the spin-flipper (> 95%) for $\lambda <$ 1.8 nm without any additional background.

Using the list mode data acquisition time-stamped measurements can be performed. Stroboscopic measurements by using a trigger signal allow for investigation of the kinetics of periodic processes. The chopper system based on TISANE technique allows for studies of microsecond dynamics.

Instrument application

- Nanoscaled materials
- Phase separation in alloys and glasses
- Morphologies of superalloys
- Magnetic correlations
- Microporosity in ceramics
- Interfaces and surfaces of catalysts
- Biological macromolecules
- Polymers and membranes
- Flux line lattices in superconductors

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

Instrument data

Neutron guide	NL 3A
Collimation	Entrance window: 50x30 mm^2 Collimator length: 2m, 4m, 8m, 12m (all also for SANSPOL), and 16m
Monochromator	Mechanical velocity selector
Wave length	$0.45 < \lambda < 2$ nm
Wave length resolution	$8\% < \Delta\lambda / \lambda < 18\%$ FWHM
Flux	$4.6 \cdot 10^6 n/cm^2$ at $\lambda = 0.5$ nm, $\Delta\lambda / \lambda = 10\%$ and collimation 2m
Q range	0.01 nm-1 < Q < 8.5 nm^{-1}
Detector	ca. 1 m diameter, 112 Reuter-Stokes tubes, 100 mm / 850 mm / 600 mm
Sample-to-detector distance	Horizontal: 1 to 16 m continuously Vertical offset: 0.17 m at short distance
Polarized neutrons	Yes
Instrument options	• SANSPOL • Stroboscopic SANS • TISANE
Sample environment	• T-controlled automatic sample changer (5°C-80°C) • Automatic sample changer with magnetic field 1.2 T
Software	BerSANS
Instrument responsible	Dr. Uwe Keiderling, keiderling@helmholtz-berlin.de

References / Latest publications

[1] Keller, T. *et al.*: The polarized neutron small-angle scattering instrument at BENSC Berlin, Nuclear Instruments and Methods in Physics Research Section A 451 (2000), 474-479.

[2] Keiderling, U., Wiedenmann, A.: New SANS Instrument at the BER II Reactor in Berlin, Germany, Physica B 213 and 214 (1995), 895-897.

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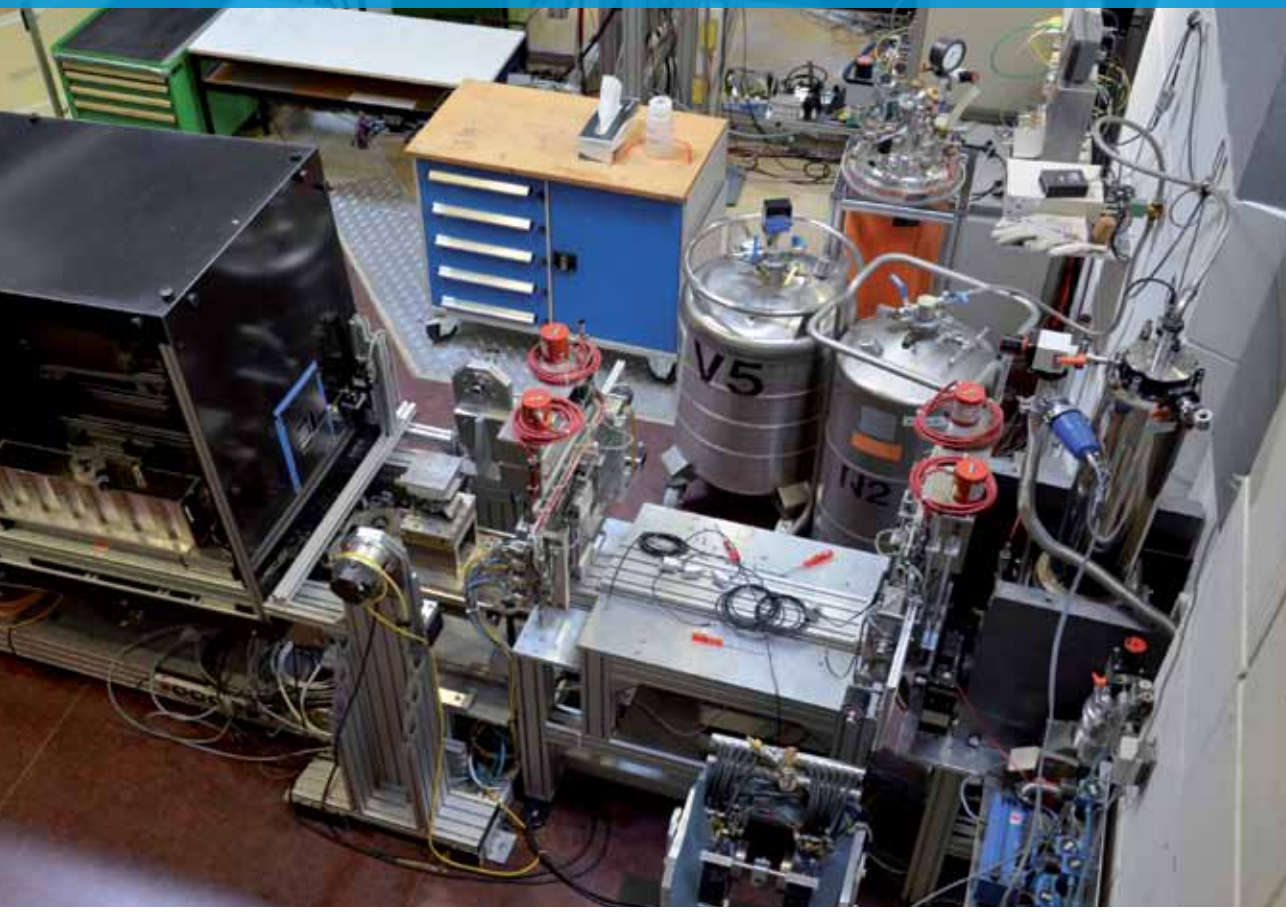
[4] Strunz, P. *et al.*: *In-situ* observation of morphological changes of g' precipitates in a pre-deformed single-crystal Ni-base superalloy, Journal of Applied Crystallography 44 (2011), 935-944.

V4 - Reference guide for latest publications

V6 | Reflectometer

The reflectometer V6 allows measuring the neutron optical reflectivities on flat surfaces at grazing angles. The reflectivity is related to the variation of the refractive index within a depth of about 200 nm, thus structural depth profiles can be studied at solid-air, solid-liquid and free liquid surfaces. Using polarized neutrons magnetic properties and magnetic depth profiles can be reconstructed in a unique way.

For solid samples the angle of incidence is varied by a precise tilting of the sample surface relative to the (fixed) collimated neutron beam. Liquid samples can also be measured. In this mode the sample surface is kept horizontal and the angle of incidence is varied by precise and synchronized movement of the monochromator tilt angle, the slit system and the sample stage. The sample-detector distance is variable between 1 m and 3 m. The instrument is capable of measuring magnetic samples with exit beam spin analysis, thus all four spin-dependent reflectivities (spin flip and non-spin flip) can be studied.



Instrument data

Neutron guide	NL 4
Collimation	2 Cd slits (computer controlled)
Monochromator	PG (002) mosaicity: $\Delta\lambda/\lambda$= 2%
Wave length	λ = 0.466 nm
Scattering plane	Vertical
Flux	$3 \cdot 10^4$ n/cm^{2}s $1.5 \cdot 10^4$ n/cm^{2}s (polarized 98.5%)
Range of reflectivities	$2 \cdot 10^5$ (with sample site 10x40 mm)
q resolution	$2 \cdot 10^{-2}$ nm^{-1} (depending on collimation)
Detector	48 ^{3}He-detector tubes Optionally multiwire PSD (180 x 180 mm, resolution 1.5 mm) Angular range: 10° (for liquids: 0° - 2.7°) Vertical collimation: 0.01° - 0.05° Angular precision: 0.001°
Polarized neutrons	Yes
Instrument options	• Solid sample mode • Liquid sample mode
Sample environment	• Sample rotation table (360°) • Heatable sample cells for air-liquid and solid-liquid interfaces • High pressure cell (100 MPa) for solid-liquid interfaces • Vacuum and gas loading cells • Langmuir film balance
Instrument responsible	Dr. Roland Steitz, steitz@helmholtz-berlin.de Dr. Beatrix-Kamelia Seidlhofer, beatrix-kamelia.seidlhofer@helmholtz-berlin.de

Instrument application

- Multilayers (inorganic or organic materials)
- Liquid and solid surfaces, solid-liquid interfaces
- Properties of in-plane structured layers
- Magnetic penetration depth in superconductors
- Magnetic properties of thin layers or multilayers
- Domain walls in spring magnet systems

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

References / Latest publications

[1] Jerliu, B. *et al.*: Neutron reflectometry studies on the lithiation of amorphous silicon electrodes in lithium-ion batteries, Physical Chemistry Chemical Physics 15 (2013), 7777-7784.

[2] Koo, J. *et al.*: Pressure-Induced Protein Adsorption at Aqueous–Solid Interfaces, Langmuir 29 (2013), 8025-8030.

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V6 - Reference guide for latest publications

V7 | Cold Neutron Tomography and Radiography (CONRAD)

V7 (CONRAD) is an imaging instrument using low energetic (cold) neutrons. The instrument is installed at the end of a curved neutron guide which blocks the direct view on the reactor core. This reflects in a very low background of high energetic neutrons and gammas. The cold neutron beam provides high attenuation contrast for thin layers of hydrogenous as well as lithium and boron based materials. In this way the visualization of small amounts of water,

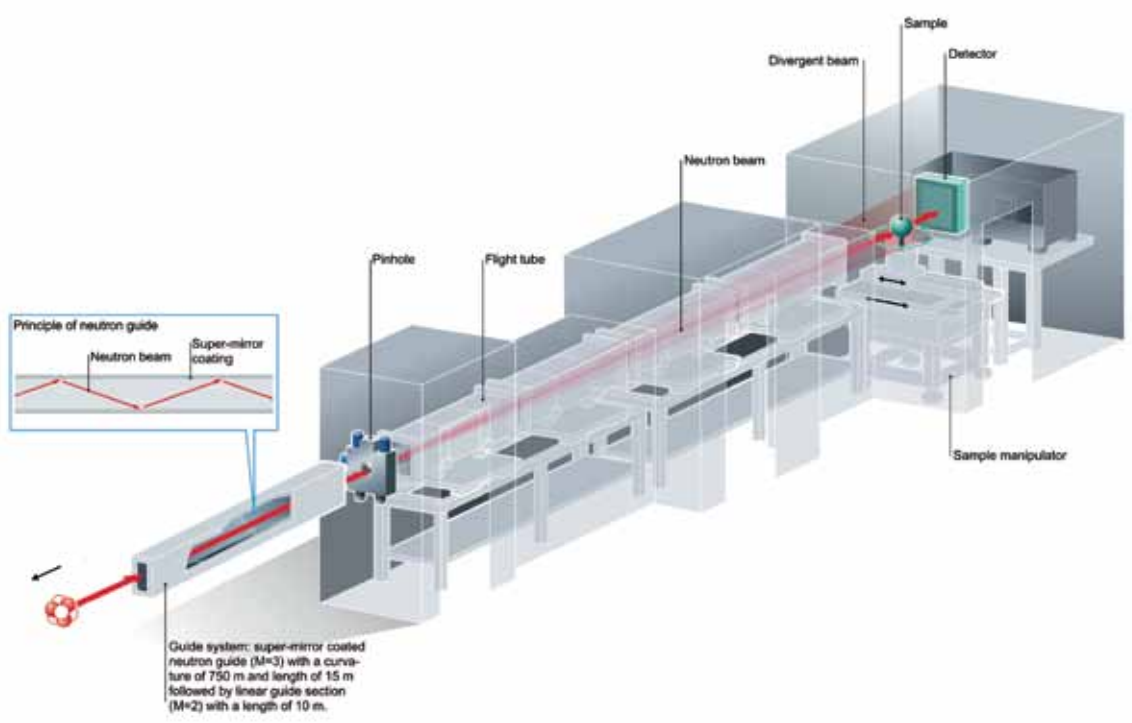
adhesive and lubricate substances in metal parts can be performed successfully. The wavelength range of the cold neutrons is suitable for phase- and diffraction-contrast imaging like grating interferometry and Bragg edge mapping. The instrument is well suited for high resolution imaging due to the high efficiency of the very thin scintillators used for cold neutrons.

Instrument application

- Energy research (fuel cells and Li-ion batteries)
- Materials research (hydrogen storage materials, phase transitions in metals and characterization of porous media)
- Life science (water uptake in plants and water management in soils)
- High-TC superconductivity (flux pinning in superconductors)
- Magnetism (visualization and analysis of domain networks and visualization of static and alternating magnetic fields)
- Cultural heritage and paleontology

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II



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V7 - Reference guide for latest publications

Instrument data

Neutron Guide	NL-1A (m=2,3) with beam cross-section: 125 mm (height) x 30 mm (width) Radius of curvature: 750 m
Pinhole changer	1 cm, 2 cm and 3 cm in diameter
Flight path	10 m flight path, covered by aluminum containers filled with He
Measuring positions	Position 1 (end of the guide) Flux: $2.6 \cdot 10^9$ n/cm²s @ L/D ca. 70; beam size: 12x3 cm Position 2 Flux: $7.2 \cdot 10^7$ n/cm²s @ L/D 170; beam size: 15x15 cm Position 3 Flux: $2.4 \cdot 10^7$ n/cm²s @ L/D 350; beam size: 30x30 cm Flux: $1.1 \cdot 10^7$ n/cm²s @ L/D 500; beam size: 30x30 cm
Double crystal monochromator	Pyrolythic graphite (002) with mosaicity of 0.8° Wavelength resolution: 3% Wavelength range: 1.5 Å – 6.0 Å
Velocity selector	Wavelength range: 3.0 Å – 6.0 Å Wavelength resolution: 10 – 20 %
Polarizers	2x Solid-state benders 4x Polarised ^{3}He cells and 2x magic boxes
Detectors	CCD camera (Andor, 2048 x 2048 pixels) sCMOS camera (Andor Neo) CMOS camera (PCO 1200h)
Best spatial resolution	20 µm at field-of-view of 13x13 mm
Sample manipulator	Rotation table: 0-360° Translation table: 0-800 mm Lift table: 0-250 mm Maximum weight: 200 kg
Instrument responsible	Dr. Nikolay Kardjilov, kardjilov@helmholtz-berlin.de Dr. André Hilger, hilger@helmholtz-berlin.de

References / Latest publications

[1] Kardjilov, N. *et al.*: Three-dimensional imaging of magnetic fields with polarized neutrons, Nature Physics 4 (2008), 399-403.

[2] Manke, I. *et al.*: Three-dimensional imaging of magnetic domains, Nature Communications 1 (2010), 125.

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[4] Schröder, A. *et al.*: In-plane neutron radiography for studying the influence of surface treatment and design of cathode flow fields in direct methanol fuel cells, International Journal of Hydrogen Energy 38 (2013), 2443-2454.

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[6] Williams, S. H. *et al.*: Detection system for microimaging with neutrons, Journal of Instrumentation 7 (2012), P02014.


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V16 | Very Small Angle Neutron Scattering (VSANS)

The second SANS instrument at BER II is dedicated to soft matter research. V16 covers a Q-range from 10^{-3} nm^{-1} to 8.5 nm^{-1}. In standard time-of-flight mode an offset of the detector to the instrument axis to extend the Q range will be possible.

The instrument works in the time-of-flight mode with ordinary pinhole collimation and in an optional low-q mode using multi pinhole grid collimation. The latter mode will allow for gravitational velocity selection and focuses many beams on a high resolution detector, only used for this option.

Instrument application

- Structure determination of mesoscopic particles (colloid particles, proteins)
- Investigation of precipitations in the range of a few nanometers to 50 nm
- Study of voids in battery electrodes (DEGAS)
- RheoSANS

References / Latest publications

[1] Vogtt, K. *et al.*: A new time-of-flight small-angle scattering instrument at the Helmholtz-Zentrum Berlin: V16/VSANS, J. Appl. Crystal. 47 (2014), 237-244.

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

Instrument data

Neutron guide	NL 4C straight behind bender, SM coated, m=1 cross section 80x80 mm^2 with cut-off λ=0.25nm
Collimation	Exchangeable pinhole and guide optics on up to 12 m length
Monochromator	TOF
Wave length	0.25 nm < λ < 1.8 nm
Q range	0.02 nm^{-1} < Q < 8.0 nm^{-1}
Q resolution	5% < ΔQ/Q < 18%, depending on the chopper settings
Detector	2D ^{3}He detector • 100x100 cm^2 area • physical pitch: 9 mm
Sample-to-detector distance	1.7m up to 11.2m
Polarized neutrons	No, but principally possible
Instrument options	• Low-Q mode (see specifics below)
Sample environment	Hellma cuvettes (120, 404), rheometer, DEGAS cell, battery cell, cryostats and magnets from sample environment group.
Software	Caress (control), Evalstat (in-house DAQ), Mantid (data reduction)
Multi pinhole mode	
Neutron guide	NL 4C straight behind bender, SM coated, m=1 cross section 80x80 mm^2 with cut-off λ=0.25nm
Collimation	Multi pinhole-grids, on 12 m length
Monochromator	Gravitational velocity selection through multi pinhole-grids
Wave length	0.25 nm < λ < 1.8 nm
Q range	0.001 nm^{-1} < Q < 0.02 nm^{-1}
Detector	2D detector with 2x3 mm^2 pitch
Instrument responsible	Dr. Daniel Clemens, clemens@helmholtz-berlin.de Dr. Miriam Siebenbürger, miriam.siebenbuerger@helmholtz-berlin.de

V16 - Reference guide for latest publications

V18 | Reflectometer for biological applications (BioRef)

BioRef is a time-of-flight reflectometer which is intended to focus on soft matter applications, especially at solid–liquid interfaces, for the investigation of biological model systems under physiological conditions including kinetic studies. The instrument was built in a joint collaboration between HZB and the University of Heidelberg with financial support by the BMBF Verbundforschung. Unique features of BioRef are the chopper system, which allows for focusing on a certain Q-range in order to support fast kinetic studies, and the availability of optional *in-situ* IR spectroscopy measurements that provide conformational information under the same experimental conditions under which simultaneously the neutron reflectivity (NR) is providing structural data.

A special feature of the instrument is an add-on sample environment that allows for simultaneous *in-situ* infrared (IR) spectroscopy of the investigated Si-supported interfaces in ATR (attenuated total reflection) geometry. A Bruker Vertex 70 infrared spectrometer is installed above the sample position for the very reason. The IR beam enters the Si substrate through the inclined top surface (45°) under 90°, is then totally reflected internally several times at the sample surface (front side) and the backside of the substrate before leaving the Si-substrate through its inclined bottom face to be deflected into the external IR-detector. The setup enables combined *in-situ* (kinetic) neutron reflectivity and IR studies with depth profile and conformational information acquired at the same time.

Instrument application

- Solid-liquid interfaces
- Combined NR and FTIR measurements
- Time resolved NR

References / Latest publications

[1] Wojciechowski, K. *et al.*: Effect of hydration of sugar groups on adsorption of Quillaja bark saponin at air/water and Si/water interfaces, Colloids and Surfaces B: Biointerfaces 177 (2014), 60-67.

[2] Kreuzer, M. *et al.*: Impact of a model synovial fluid on supported lipid membranes, Biochimica et Biophysica Acta (BBA) - Biomembranes 1818 (2012), 2648-2659.

[3] Strobl, M. *et al.*: A versatile time-of-flight reflectometer for soft matter applications at Helmholtz–Zentrum Berlin, Review of Scientific Instruments 82 (2011), 055101.

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NEUTRON GUIDE
HALL BER II

INSTRUMENTS
BER II

V18 - Reference guide
for latest publications

Instrument data

Neutron guide	NL 3b
Wave length	90 Hz: 2.0 - 6.0 Å 45 Hz: 2.0 - 10.0 Å 25 Hz: 2.0 - 16.4 Å
Wave length resolution	Constsnt $\Delta\lambda/\lambda$= 1 -5%, 7% - 11%
Scattering plane	Horizontal
Range of reflectivities	$1x10^{-7}$ with a 50x80 mm^2 sample
Q resolution	$\Delta Q/Q$ = 1.4 – 7% and 10 – 15%
Detector	300 x 300 mm^2 Multiwire PSD detector
Polarized neutrons	No
Instrument options	Posibility of combined NR and ATR-IR measurments
Sample environment	Rectangular flow cells (50x80 mm^2) Round flow cells (∅ 60mm) Hydration chamber
Instrument responsible	Dr. Marcus Trapp, marcus.trapp@helmholtz-berlin.de Dr. Beatrix-Kamelia Seidlhofer, beatrix-kamelia.seidlhofer@helmholtz-berlin.de

B8 | Neutron-Autoradiography

The instrument B8 allows to irradiate and activate artistic, technical, or geological items (foils, stones etc.) and other materials with cold neutrons and to investigate it afterwards with imaging plate technique and/or to analyse it with γ-spectroscopy. The painting is fixed on a support in front of a neutron guide end with an open area of 3.5 x12.5 cm^2. The surface of the painting is adjusted under a small angle (< 3°) with respect to the axis of the guide so that the main free path of the neutrons within the paint layer is much longer than in the case of perpendicular transmission. The support is moved up and down with a velocity of a few cm/s in order to receive a uniform activation of the total area of the panel.

On a special table in a shielded room in the basement the film exposure and the gamma spectroscopy can be performed for the suitable times (up to more than 4 weeks) depending on the half-lives of the isotopes.

- Activation cross-section (n,β) depends on the isotope
- Different pictures depending on the half-lifetimes of the isotopes
- Less γ-rays (cold source)
- Non-destructive

Instrument data

Neutron guide	NL 1a
Wave length	white beam (cold spectrum)
Neutron flux	10^9 n/cm^{2}s
Instrument responsible	Dr. Andrea Denker,denker@helmholtz-berlin.de

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

Instrument application

- Autoradiography of paintings
- γ-spectroscopy of coins
- Irridiation

Application of autoradiography to paintings

After irradiation, the neutron-induced radioactivity decays with time. About a dozen different light and heavy isotopes – emitting β- (electrons) and γ-radiation – are created (the most important isotopes and their half-lives are presented in table 1). The induced β-decay is used to blacken highly sensitive films or imaging plates to reveal the spatial distribution of the pigments. It is a big advantage of neutrons that different pigments can be represented on separate films. This is due to a contrast variation created by the differences in the half-life times of the isotopes.

Isotope	Half life	Pigment
^{56}Mn	2.6 h	Brown colours, Umber, Ocre
^{64}Cu	13 h	Azurite, Malachite
^{76}As	1.1 d	Smalt, Realgar, Auripigmente
^{122}Sb ^{124}Sb	2.7 d 60 d	Naples-Yellow
^{32}p	14 d	Bone-black
^{203}Hg	47 d	Vermilion
^{60}Co	5.3 a	Smalt

The γ-spectroscopy via a Ge-detector provides information about the element composition of the pigments. The image plate technique allows for direct digital analysis and processing. With this method conceptual changes and corrections (“pentimenti”) during the creation of the painting become visible. In some cases decisions about the authenticity can be made. The art historian or restorer receives valuable information about the brush technique of the artist and the actual condition of the painting.

References / Latest publications

[1] Denker, A.: Analysis of 51 selected coins at the Helmholtz-Zentrum Berlin für Materialien und Energie, In: Mahlo, D. [Ed.]: The early coins of Myanmar/Burma: messengers from the past ; Pyu, Mon, and Candras of Arakan (first millenium AD). Bangkok: White Lotus Press, (2012) - ISBN 978-974-480-191-3, 149-152.

[2] Denker, A. *et al.*: The genesis of Jan Steens painting "As the old ones sing, so the young ones pipe" from the Gemäldegalerie Berlin, Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 651 (2011), 273-276.

B8- Reference guide for latest publications


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HZB Helmholtz Zentrum Berlin

BER II

CRG Instruments

V12a | Beuth
Bent-crystal Diffractometer (USANS) with Tomography option

An asymmetrically cut perfect Si single crystal monochromator is located is deflecting neutrons of 4.76 Å by (111) Bragg diffraction towards the sample position and the downstream end face of a completely asymmetrically cut analyzer crystal. The asymmetry of the monochromator (α = 41°) changes the beam cross section from 3 x 5 cm^2 of the guide to 0.5 x 5 cm^2 at the sample side. After penetrating and interacting with a sample the beam passes a 0.3 x 2 cm^2 slit, enters the bent perfect Si single crystal analyzer and propagates along its long side. At the spot in the crystal, where the Bragg condition is satisfied, neutrons are deflected through the long side of the crystal towards the position sensitive detector. Neutrons which were scattered by an interaction in the sample will be deflected at a different spot in the analyzer and hence are registered in a different part of the detector than without interaction. By comparison with the empty beam scattering angles of the order of seconds of arc can be resolved on an angular range up to 0.5°.

V12 is complementing small angle scattering machines on the low angle side with overlapping q-ranges. Furthermore equipped with a 2-dimensional position sensitive detector spatial resolved USANS investigations and even tomographies can be performed.

Instrument application

- Porous materials (*e.g.* cement, paste, rocks, coal etc.)
- Particles and inhomogenities on a size range from 50 nm to 10 µm
- Artificial regular structures (*e.g.* phase gratings)
- Magnetic domains (*e.g.* Bloch walls)

Instrument data

Neutron guide	NL 3B
Monochromator	Perfect Si single crystal (111), edged, asymmetric alpha
Wave length	λ = 0.476 nm
Flux	$2 \cdot 10^3$ n/cm^{2}s
Q range	10^{-3} nm^{-1} < Q < 10^{-1} nm^{-1}
Q resolution	$\Delta Q/Q = 1.5 \cdot 10^{-4}$ nm^{-1}
Polarized neutrons	No
Instrument options	• Spatial resolved USANS (using 2D PSD) • Tomography
Diffraction analyser crystals	Perfect Si single crystal (111), edged, completely asymmetric
Instrument responsible	Prof. Wolfgang Treimer, treimer@helmholtz-berlin.de MSc Nursel Karakas, nursel.karakas@helmholtz-berlin.de

References / Latest publications

[1] Strobl, M. *et al.*: Small angle scattering signals for (neutron) computerized tomography, Appl. Phys. Let. 85 (2004), 3, 488.

[2] Treimer, W. *et al.*: Refraction as imaging signal for computerized (neutron) tomography, Appl. Phys. Let. 83 (2003), 2, 398.

[3] Gravey, C.J. *et al.*: Small angle neutron scattering on an absolute intensity scale and the internal surface of diatom frustules from three species of differing morphologies, European Biophysics Journal with Biophysics Letters 42 (2013), 395-404.

[4] Raitman, E. *et al.*: Propagation of neutron spherical waves through a thick, vibrating Ge single crystal, Acta Crystallographica Section A 69 (2013), 189-196.

Additional Publications

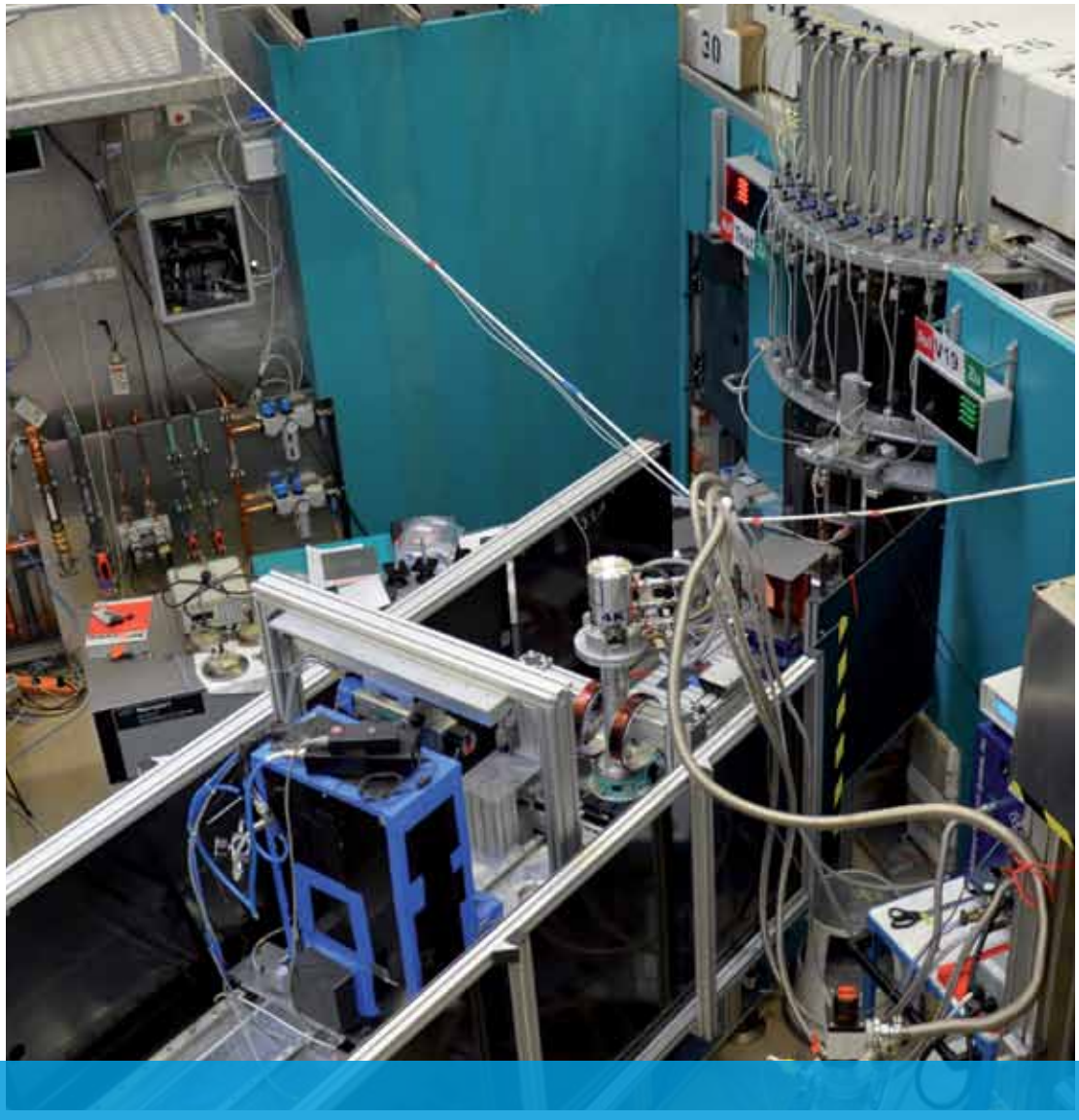
Garvey, C. J. *et al.*: Small angle neutron scattering on an absolute intensity scale and the internal surface of diatom frustules from three species of differing morphologies, European Biophysics Journal with Biophysics Letters 42 (2013), 395-404.

Raitman, E. *et al.*: Propagation of neutron spherical waves through a thick, vibrating Ge single crystal, Acta Crystallographica Section A 69 (2013), 189-196.

NEUTRON GUIDE HALL BER II

INSTRUMENTS CRG BER II

V12a- Reference guide for latest publications



V19 | Beuth
Polarized Neutron Tomography (PONTO)

PONTO is an instrument dedicated to high resolution radiography and tomography with polarized neutrons. The combination of a graphite crystal as monochromator and two crossed collimations yields an equivalent L/D – ratio of 570, which is constant for all source – sample distances. This allows for very flexible and different samples environments a constant spatial resolution of 60 µm (un-polarized) and < 150 µm (polarized neutrons). Beside this, it is characterized by a high beam polarization P ~ 96% and vey homogenous field of view (40 mm x 40 mm).

Instrument data

Wave length	0.30 < λ < 0.45 nm
L/D	570
Resolution	unpolarized: 60 µm / polarized : < 150 µm
Exposure time	5‘ - 120‘
Beam size	40 mm x 40 mm
Detector	2k x 2k
Software	VG Studio, COMSOL Multiphysics, Octopus 3D viewer, National Instruments LabView, Mathlab, Mathcad
Instrument responsible	Prof. Wolfgang Treimer, treimer@helmholtz-berlin.de Dipl.Ing. M. E. Omid Ebrahimi, omid.ebrahimi@helmholtz-berlin.de

Instrument application

- Radiography and tomography with polarized neutrons
- Superconductors
- Flux trapping
- Meissner effect
- Small magnets
- Magnetic phase transitions

NEUTRON GUIDE HALL BER II

INSTRUMENTS CRG BER II

References / Latest publications

[1] Treimer, W. *et al.*: Neutron tomography using a crystal monochromator, Nuclear Instruments and Methods in Physics Research A 621 (2010), 502-505.

[2] Aull, S. *et al.*: Suppressed Meissner-effect in Niobium: Visualized with polarized neutron radiography, Journal of Physics, Conf. Series 340 (2012), 012001.

[3] Treimer, W. *et al.*: Polarized neutron imaging and 3D calculation of magnetic flux trapping in bulk of super-conductors, Phys. Rev. B 85 (2012), 184522.

[4] Treimer, W. *et al.*: Observation of partial Meissner effect and flux pinning in superconducting lead containing non-superconducting parts, Appl. Phys. Lett. 101 (2012), 162603.

[5] Treimer, W. *et al.*: Imaging Quantum Mechanical Effects in Superconductors with Polarized Neutrons, Physics Procedia 42 (2013), 31-38.

[6] Treimer, W. *et al.*: Imaging of Quantum mechanical effects in superconductors by means of polarized neutron radiography, Physics Procedia 43 (2013), 243-253.

[7] Treimer, W.: Radiography and tomography with polarized neutrons, J. Magn. Magn. Mater. 350 (2014), 188-198.

V19 - Reference guide for latest publications

BER II

Projects


HZB
Helmholtz
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V3 | Time-of-flight neutron Spectrometer (NEAT)

The cold neutron chopper spectrometer NEAT at Helmholtz-Zentrum Berlin is best suited to probe dynamic phenomena directly in space and time in the time domain 10^{-13} – 10^{-11} s and on the length scale ranging from microscopic (0.5 Å) to nanoscale dimensions (up to about 50 nm). Hence the spectrum of application is very broad, ranging from the lattice dynamics in semiconductors to the transport phenomena in energy storage systems and spin dynamics in high-Tc superconductors. Currently NEAT is undergoing an upgrade with the goal to achieve the substantial increase of intensity and implementation of new capabilities. NEAT will have an access to very large wavelength range of 2-20 Å with variable energy and angular resolution. The advanced features of the new instrument include novel neutron guide system with exchangeable focusing sections to adapt best to the samples of various sizes.

A new design of the chopper system is a substantial improvement that allows to double flux at high resolution conditions. The instrument design foresees the application with variable sample environment including high-field magnet of 15 T. Novel position sensitive detectors will cover a large solid angle of 270° and allow for the single crystal applications. The project started in 2010 and proceeds at full pace with the aimed start of the commissioning. The new instrument will provide an outstanding experimental tool for a large spectrum of research areas ranging from hydrogen storage matter, to solar cells and to materials for quantum information technology.

Instrument application

- Materials for energy storage and conduction: hydrogen storage systems, high capacitors, novel electrolytes, ionic liquids, ionic conducting systems and etc.
- Confinement phenomena in magnetism and soft matter
- Spin dynamics in high-T_C-superconductors,
- Molecular magnets, quantum magnetism phenomena
- Dynamics of biological systems and soft matter, including proteins, membranes, and hydration water etc.
- Lattice dynamics and transport phenomena in novel semiconducting materials
- Systems under extreme sample environment: high pressure, high magnetic field, low and high temperatures.

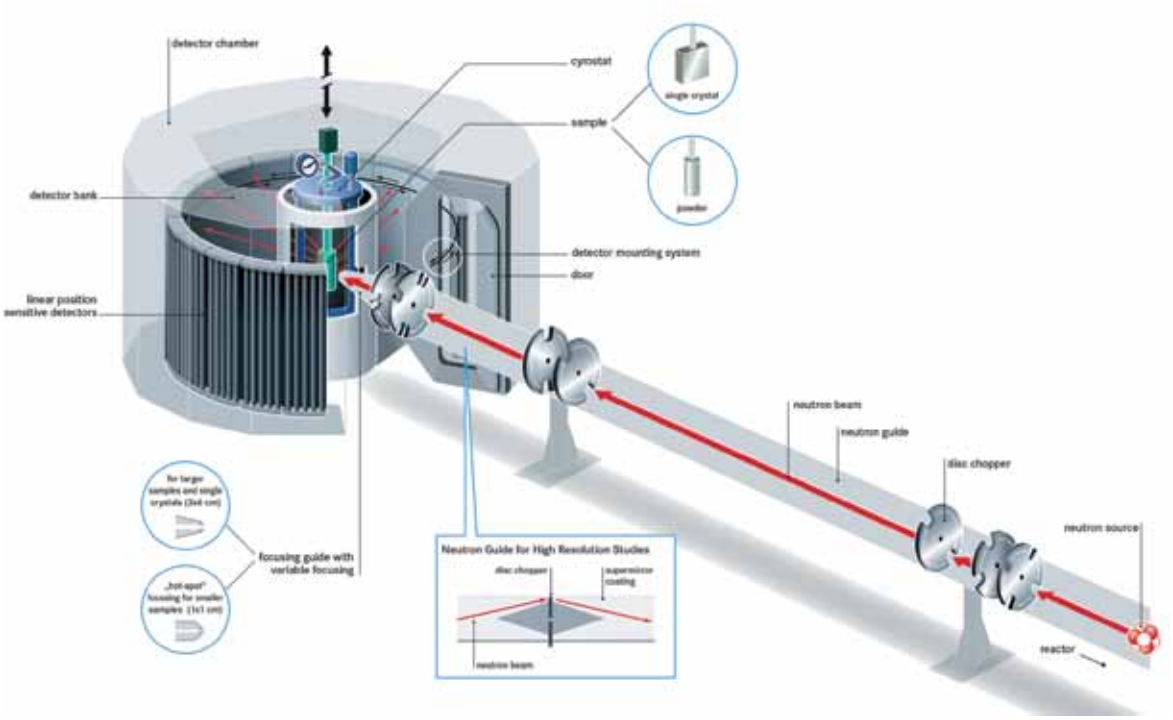
References / Latest publications

[1] Peterson, V. *et al.*: Superfast Proton Diffusion in a Plasma-Polymerized Fuel-Cell Membrane studied by Time-Of-Flight neutron spectroscopy, J. Phys. Chem. C 117 (2013), 4351-4357.

[2] Podlesnyak, A. *et al.*: Origin of spin state polaron in doped perovskite materials, Phys. Rev. Lett. 101 (2008), 247603.

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II



Instrument data

Neutron guide	NL-2new
Beam cross section at the sample	30 x 55 mm, 20 x 20 mm
Chopper slits	Two pairs, optimized for hard and soft matter studies
Distance between choppers (1,2) and (6,7)	30 m
Distance from the last chopper to the sample	1.30
Chopper speed range	Up to 20000 rpm
Incident wavelength range in the monochromatic mode	0.18 nm – 1.9 nm
Elastic energy resolution (FWHM) at SD	6 meV – 5400 meV
Range of scattering angles	-142° - 70°
Distance from sample to SD	3 m
Sample environment	Cryofurnace (⌀ 80 mm): 1.5-570 K Dilution stick: 0.1 -1 K ^{3}He-insert: 0.4 - 40 K HT-furnace (⌀ 70 mm): 300-1270 K Magnetic field: 15 T High pressure: 3 kbar (gaseous) *In-situ* laser illumination
Instrument responsible	Dr. Margarita Russina, margarita.russina@helmholtz-berlin.de

V3 - Reference guide for latest publications

HFM/EXED | High Magnetic Field Facility for Neutron Scattering

The Extreme Environment Diffractometer (EXED) is a time-of-flight instrument optimized for diffraction in restricted angular geometries typical for extreme sample environment. A special focus is on neutron scattering in high magnetic fields. In the near future the instrument will be furnished by a dedicated 25+ T High Field hybrid Magnet (HFM), currently being built by the HZB in collaboration with the National High Magnetic Field Laboratory (Florida, US).

The instrument

EXED is equipped with a multispectral extraction system followed by about 70 m long supermirror guide. As a result, neutrons from both thermal and cold moderators with wavelength range from 0.7 to 15 Å are available for experiments. The lower wavelength limit is given by the kink in the guide that blocks the direct view of the source and provides a sharp cut-off. Apart from the kink, the guide is essentially straight (100 x 60 mm^2 (HxW)) and ends with an elliptic focusing section that compresses the beam spatially in both directions by a factor of 2. For applications requiring low beam divergence, the focusing end can be replaced by a 6 m long pin-hole collimation section with variable apertures. Flexibility of the instrument is ensured by three alternative systems that are available to create neutron pulses: a curved Fermi chopper for very high resolution (Δt ~ 6 µs), a straight Fermi chopper for high resolution (Δt ~ 15 µs) and a counter- or parallel-rotating double disk chopper for medium to low resolution (from 115 µs up to >5000 µs). A number of single disk choppers located downstream prevents frame overlap and defines the bandwidth of interest. Due to the chopper system one can operate the instrument from narrow (~ 0.6 Å) to wide (~ 14.4 Å) wavelength band mode centered at the region of interest, and easily trade resolution for intensity. The secondary instrument is equipped with position-sensitive ^{3}He detector tubes. They are combined in 4 movable detector banks that can be positioned at different angles around the sample. While the typical sample-detector distance is 1.2 m, a large He-filled detector chamber allows positioning of two detector panels at 6 m away from the sample. In its current configuration (*i.e.* w/o HFM) EXED has no angular restrictions and can be used with all types of standard sample environment available at HZB, as well as user own equipment. It complements HZB's diffraction instrument suite by providing characteristics typical for pulsed instruments *e.g.* high resolution in backscattering ($\Delta d/d > 10^{-3}$) and large dynamic range (0.5 - 1000 Å). Event-recording data makes time-resolved measurements readily available.

Operation Modes of EXED+HFM

In order to enable a broad range of scientific applications using unique combination of neutron scattering and high magnetic fields, EXED is being currently upgraded. A novel concept will combine several scattering techniques in one instrument. The operation modes of multi-purpose EXED are described below.

Elastic (available from the "day one" of combined HFM/EXED operation): Primarily built as a diffractometer, EXED will maintain this option while significantly expanding the low Q-range accessible for the experiments. In its low-Q mode momentum transfer down to 10^{-2} Å will be accessible using a 6m-long collimation combined with 6m-long He-filled detector chamber. The latter will enable studies of matter on nanoscales in high magnetic fields such as *e.g.* vortex state in type-two superconductors.
Both single crystal and powder diffraction will be possible. Performed in the same manner as at present. Upgrade for the inelastic mode (details are given below) will result in further improvement of the elastic performance (signal-to-noise ratio and full angular coverage in forward scattering).

Inelastic (under development): A major development is taking place to complement the instrument portfolio by inelastic capabilities in the form of a direct TOF spectrometer. The upgrade includes four main components: i) a detector chamber for forward scattering with a built-in ii) ^{3}He detector array covering 30° in- and out- of plane and positioned 4.5 m away from the sample, and iii) a new focusing guide section that accommodates iv) a monochromating chopper assembly. The chopper produces short monochromatic neutron pulses and TOF is used to analyze the change in the energy of the scattered neutrons. Limited sample size inside the HFM and weak inelastic scattering cross sections imply the need for optimization for signal strength and low-background conditions. The former is achieved by enhancing the flux at the sample using a novel focusing guide, while the latter is provided by means of a shielded and evacuated detector chamber. After completion, the upgraded EXED will enable energy-resolved measurements over a limited Q-range $< 3.25/\lambda(Å^{-1})$ in addition to the existing elastic capabilities.

-> please continue on the next page

NEUTRON GUIDE HALL BER II

INSTRUMENTS BER II

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Instrument data

Beam tube	NL 4A, 75 m long ballistic multispectral guide 60 x 100 mm^2 (straight section) elliptically tapered down to 30 x 50 mm^2 (7.5 m long focusing section)
Collimation	i) None (standard configuration) ii) 6 m long pin-hole collimation section can replace focusing section
Wave length	$0.7 < \lambda < 15$ Å
Flux	~ $1.5 \cdot 10^9$ n/cm^2s - continuous flux
Range of scattering angles	i) Without HFM ±0-170° ii) With HFM Elastic 0 – 30°, 150° – 170° Inelastic 0 – 30°
Range of lattice spacing	Forward scattering: $2 < d < 1000$ Å Backward scattering: $0.5 < d < 7$ Å
d resolution	Forward scattering: $\Delta d/d > 2 \cdot 10^{-2}$ Backward scattering: $\Delta d/d > 1 \cdot 10^{-3}$
Sample size	i) Without HFM 2x4 cm^2 (WxH) ii) With HFM <1.5x1.5 cm^2
Detector	192 ^{3}He linear position sensitive detectors combined in 4 sections, each containing 48 detector tubes of 90 cm effective length and ½" diameter
Instrument options	Elastic: Powder and Single Crystal Diffraction; Low Q Inelastic: under development (direct TOF spectrometer)
Sample environment	i) Without HFM T = 0.05 – 600 K, B ≤ 17 T ii) With HFM T = 0.5 – 300 K, B = 25+ T (horizontal field)
Software	egraph (event recording data reduction), Mantid (data reduction)
Chopper speed range	5 – 600 Hz (Fermi chopper) 5 – 215 Hz (double disc choppers) 5 – 120 Hz (single disc choppers)
Sample-detector distance	i) Without HFM 1.2, 6 m ii) With HFM 2.5 - 4.5 m
Instrument responsible	Dr. Oleksandr Prokhnenko, prokhnenko@helmholtz-berlin.de Dr. Wolf-Dieter Stein, wolf-dieter.stein@helmholtz-berlin.de Dr. Maciej Bartkowiak, maciej.bartkowiak@helmholtz-berlin.de

Instrument application

- Quantum magnets and quantum phase transitions
- Superconductivity
- Correlated electrons in 3d, 4f and 5f metal compounds
- Spin, charge and lattice degrees of freedom in transition metal oxides
- Frustrated magnets
- Novel states of matter

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[1] Prokes, K. *et al.*: Antiferromagnetic ordering in a mixed-valent cerium compound CeRuSn, Phys. Rev. B 87 (2013), 094421.

[2] Habicht, K. *et al.*: Instrument Development for Spallation Neutron Sources Carried out at the Helmholtz-Zentrum Berlin, Neutron News 22 (2011), 36-40.

[3] Prokes, K. *et al.*: Extreme Environment Diffractometer (EXED) delivers first scientific results, Neutron News 21 (2010), 32-33.

The High Field Magnet

The HFM is a „first of its kind“ hybrid magnet system which is capable to reach fields between 25 T and 32 T, making it by far the strongest continuous field available for neutron scattering experiments worldwide (see HFM data Table). The HFM utilizes Series Connected Hybrid System Technology where water cooled resistive insert coils are mounted in the room temperature bore of a superconducting cable-in-conduit solenoid. Operation of the magnet system requires a dedicated technical infrastructure consisting of high-pressure water cooling for the resistive coil, 4 K Helium refrigerator for cooling of the superconducting coil and 20 kA DC power supply. For the moment all the magnet infrastructure components have been successfully tested and commissioning of the magnet system has started in 2014.

As the field is horizontal, a special feature of the HFM is 30° degrees conical openings at both ends of the resistive insert envisaged for neutron-scattering access. Rotating the magnet by 15° with respect to the incoming beam will result in $2q_{max}$=30° in forward scattering. A dedicated ^{3}He cryostat will allow high-field experiments to be combined with temperatures down to 0.5 K on samples <1.5 x 1.5 cm^2.

Central Field	> 25 T
Bore	50 mm horizontal, warm bore
Opening Angle	30°
Power Resistive Insert	4.4 MW
Field Homogeneity	< 0.5% Cyl. 20 mm Ø 20 mm length
Operating Current	20 kA
Magnetic Field of Resistive Insert	12 - 13 T (4.4 MW)
Magnetic Field of Supercond. Coil	12 - 13 T
Height	~ 5 m
Total Weight	~ 25 t
Cold Mass (4.5 K)	~ 6 t

User Lab Cluster


HZB
Helmholtz
Zentrum Berlin
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Sample Environment

A broad range of equipment is available to provide different sample environments for neutron scattering experiments with a wide temperature range, T = 30 mK - 2000 K, with variable magnetic fields up to H = 17 Tesla and with pressure up to p = 10 kbar. The components are mutually compatible and can be used on most of the instruments both in the experimental and the neutron guide hall.

- Magnet Cryostats with Vertical Field, Temperature range: 1.5 – 500 K, Magnetic field: 4.2 – 14.8 T
- Magnet Cryostats with Horizontal Field, Temperature range: 1.5 – 300 K, Magnetic field: 4.0 T
- Low Temperature Cryostat & Inserts, Temperatur range: 40 mK – 300 K, Thermometry Sensors: RuO_2, Cernox
- Controlled Gas Atmospheres / Adsorption Inserts, Cryostat, and Gashandlings, Pressure Range: 1 GPa, Temperature range: 1.5 – 1300 K
- High Pressure Cells, Pressure Range: 1.5 GPa at 300 K, Temperature range: 40 mK – 300 K
- LaMMB InSitu Measurements
- Soft Matter Equipment, Min. Temperature: 250 K, max. Temperature: 350 K
- Special Inserts and Sample Sticks, Temperature range: 1.7 – 550 K
- Orange Cryostats, Temperature range: 1.4 – 600 K, Thermometry Sensors: RhFe
- Closed Cycle Refrigerators, Temperature range: 4 – 450 K, Thermometry Sensors: RhFe, Si-Diode, Cernox
- High Temperature Furnaces, Temperature range: 400 – 2000 K
- Dry Cryostats, Temperature range: 1.5 – 600 K, Thermometry Sensors: Cernox

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Dr. Dirk Wallacher,
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Sample Environment - Reference guide for latest publications

BioLab

The BioLab is an essential service unit for the HZB user platform and provides on-site sample preparation and characterisation in parallel and complementary to neutron and X-ray scattering experiments. It is routinely used by users with the scientific background soft matter and biology, a community of 1/3rd of all users.

The BioLab offers a broad range of laboratory-based equipment with a focus on methods in optical spectroscopy. Specialised sample environments for neutron scattering experiments, especially complementary to neutron diffraction and reflectometry, SANS, SAXS, INS and QENS are developed. The expertise ranges from membrane biophysics and structural biology over protein dynamics to structure and function of interfaces.

Significant achievements for the user support are sophisticated preparation methods for model membranes, a reliable and robust protocol for the preparation of “free floating bilayers” for neutron reflectivity, and a novel real-time (laser-neutron) pump-probe experiment to study modulation in protein dynamics by neutron scattering methods.

Equipment

- Absorption- and fluorescence spectroscopy
- Laser laboratory with ns time resolved spectroscopy
- Fluorescence microscopy
- Langmuir balances
- ATR-FTIR spectroscopy
- Dynamic light scattering

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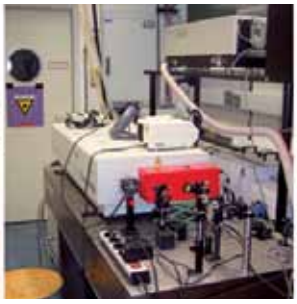

BioLab - Reference guide for latest publications



Chemistry Lab

The chemistry lab has all the facilities for the synthesis and the characterization of colloidal suspensions, supramolecular structures as well as hybrid materials for energy storage. The main task of chemistry lab is to give support for the users during their beam time in HZB. This includes not only supporting the user with full-equipped chemistry and electrochemistry lab for sample preparation, but also providing the service of basic characterization of the samples (such as electrochemical measurements, auto-titration, zeta-potential etc.) as well as cryo-TEM measurement service to the users (long term). All the synthesis labs and sample preparation labs are equipped with fume hoods. Special requirement for the preparation of samples in glovebox is also possible during beamtime. In addition, we supply users with professional guide for synthesis of different colloidal particles (from organic to inorganic particles).

The combination of user service and professional technical support based on colloid chemistry provides an important research concept in the Institute of Soft Matter and Functional Materials. Special research interests are focused on the design and fabrication of functional hybrid materials based on colloidal particles with versatile applications, such as lithium batteries, catalysts and solar cells.

The Chemistry lab locates in the Wannsee campus, which includes:
- Sample preparation lab (V108, UYH0343)
- Synthesis lab (L130, L131)
- Electrochemistry lab (LS224)
- Sample purification lab (LS123)
- Cryo-TEM (long term)

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Chemistry Lab - Reference guide for latest publications

Colloid Lab

As a general rule, our equipment shall be available for guest groups, especially those scientists that have been granted beam time on the neutron or synchrotron instruments to allow for a complete and proper characterization of their samples. This opportunity is another manifestation of HZB's mission to offer "neutrons and more" to the users, which includes the support by the scientific and technical staff. Similarly to the regulations for the large scale research instruments, the access to the laser lab is subject to safety instructions prior to access. With these facilities we are near to a complete park of tools for the characterization of colloidal suspensions, micelles, and supramolecular structures generated in aqueous suspension.

The colloid lab hosts equipment for studies to measure physical parameters, complementary to the proposed experiments at the neutron and X-ray user instruments. It also serves HZB scientists in their daily "in-house" research. The lab is run by the colloid physics group within the Institute for Soft Matter and Functional Materials. The available laboratory methods comprise thermally controlled static and dynamic light scattering (SLS/DLS/DDLS). Both are situated in our large class IIIb laser laboratory (LS117) together with a commercial Malvern Zeta-Sizer.

Additionally we run three rheometers in a dedicated lab (LS217), one of which is foreseen to be adapted to the small-angle neutron scattering instrument V16. The group research on mesoscopic materials as colloidal suspensions, micelles and supramolecular structures is in this way fully cross-linked with the development of instruments as well as the accessibility to and service of supporting laboratory equipment.

Depending on the state of an accepted proposal, either short term or long term, we offer reduced (DLS, Zeta sizer) or full (+SLS, DDLS) access to our light scattering equipment. The corresponding table shall give an overview about the parameters of our light scattering spectrometers.

As another class of experiments that may be supported by lab experiments we offer for long term proposal users to benefit from our rheology instruments. This shall primarily complement the Rheo-SANS experiments on the VSANS instrument in order to couple structural data to rheological data.

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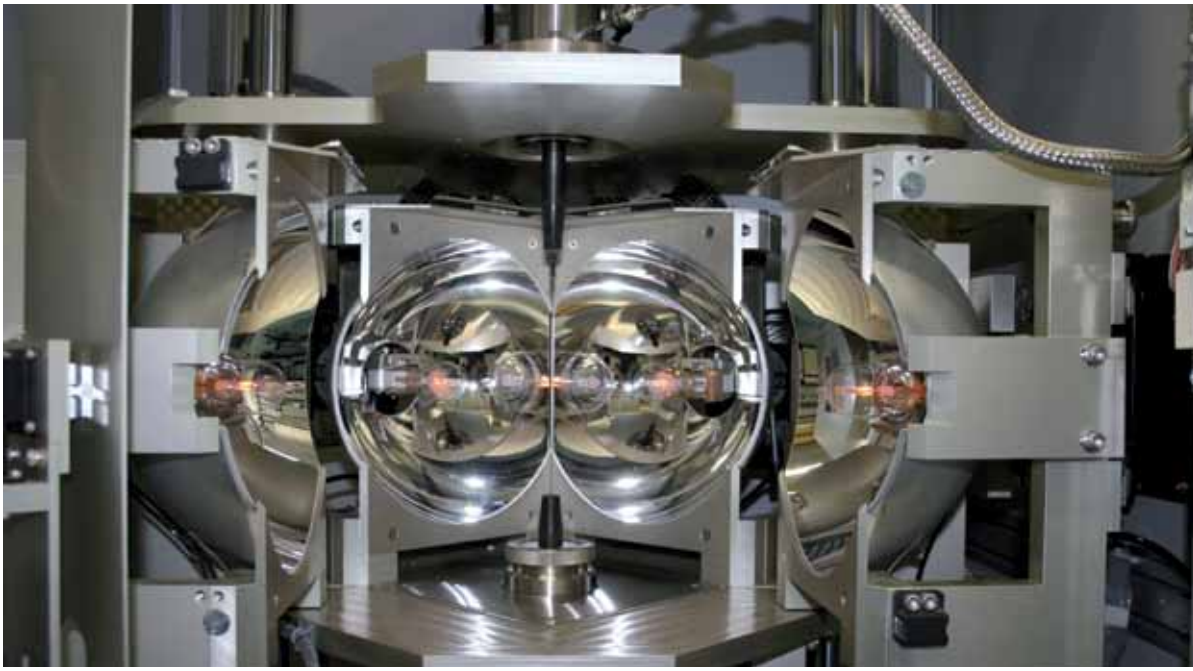
Colloid Lab - Reference guide for latest publications



Crystal Lab

The Crystal Lab suite integrates chemical instruments and methods necessary to synthesize novel materials. Typical materials are new low dimensional magnets or substances which are technically important, *e.g.* superconductors, multiferroics or thermoelectrics.

We provide many methods to control the material synthesis from the initial constituents to the final products – the samples for our research at HZB. Important are high temperature furnaces where up to 3000°C can be reached using different gas atmosphere.

The access to the Crystal Lab is open for members of the HZB. The resources are accessible through the booking system. Users will be trained so that they are able to follow their synthesis plans independently. We also welcome external users, but the contact must be mediated by members of the HZB.

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Crystal Lab - Reference guide for latest publications

DEGAS | Laboratory for Gas Adsorption Measurements at HZB

In 2006 the Hahn-Meitner-Institute Berlin started establishing a dedicated sample environment (DEGAS), answering the strongly increased requests on neutron scattering experiments combined with in-situ gas adsorption measurements. Due to the complexity of sample preparation and characterization in this type of investigations, it appeared reasonable to offer the suite of the modular experimental setups also for preliminary and completing measurements "off-beam" in the laboratory.

Up till now more than 10 different gas-adsorption modules cover a wide pressure and temperature range from 4 K to 1500 K and pressures up to 10000 bars. Thereby volumetric as well as gravimetric controlled sample loading can be combined with stepwise and continuous gas dosing methods.

The DEGAS laboratory is open for internal and external scientist, if their projected investigations contribute to the preparation or completion of neutron or X-ray scattering research at the Helmholtz Centre Berlin or related facilities. A web-based reservation system for the laboratory is actually under construction.
BER II instrument responsibles can access of the DEGAS equipment for scheduled neutron scattering experiments combined with *in-situ* gas adsorption via the sample environment booking calendar.

Contact: Dr. Dirk Wallacher,
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DEGAS - Reference guide for latest publications

LaMMB – MagLab | Laboratory for Magnetic Measurements

Since recent years, the Institute for Complex Magnetic Materials and the Sample Environment Group operate a variety of research laboratories for sample characterisation. In order to install a service for users providing access to complementary measurements at extreme conditions, these laboratories have been combined to form the new Laboratory for Magnetic Measurements (LaMMB - MagLab).

At present, the possibilities of LaMMB - MagLab offer four fully operating measurement systems with magnetic fields up to 14.5 T and temperatures down to 260 mK. The available measurement options are heat capacity, heat conduction, magneto-caloric effect, magnetisation and resistivity. Other measurement options like the dielectric constant measurement, electric polarization measurements or the cantilever magnetometer are presently under construction. In the near future a new state-of-the-art cryogenic system with magnetic fields up to 17 T and temperatures down to below 10 mK will greatly extend the temperature and magnetic field range of the measurements at LaMMB - MagLab.

The access to the LaMMB - MagLab experiments is organized via the LaMMB - MagLab booking calendar. To apply for measurement time please click on the desired instrument or the desired day and fill in the form. The request will then be forwarded to the LaMMB - MagLab instrument responsible. Presently the experiments can be booked only by members of the Helmholtz Zentrum Berlin. The access for external scientists has to be mediated by an in house scientist. Please contact the LaMMB - MagLab instrument responsibles or any of the LaMMB - MagLab staff.

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LaMMB - MagLab - Reference guide for latest publications

3D Lab |
Laboratory for analysis of volumetric 3D data

Laboratory description

The 3D Analytics Laboratory supports users performing imaging experiments at the large scale facilities at HZB. The laboratory is used for complex 2D and 3D analyses of tomographic experiments carried out at the neutron imaging instrument CONRAD-2, in the X-ray Tomography Lab (Micro-CT Lab) and at the synchrotron tomography instrument at BESSY. The 3D Analytics Laboratoryconsists of a cluster of powerful work stations equipped with state-of-art software for tomographic reconstruction and quantitative analysis of 3D data. In addition, innovative software developed in-house is provided to the users.

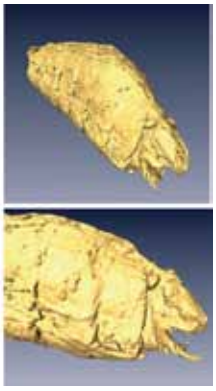
Laboratory application

- Tomographic reconstruction with innovative mathematical algorithms (parallel beam, cone beam, filtered back projection, etc.)
- Holotomographic reconstruction algorithms (phase retrieval)
- Complex 3D image analysis procedures: labelling and individual particle size and shape analysis; Euclidian distance transformations; Watershed analysis and many others.

Examples:

- Energy research (*e.g.* quantitative analysis of particles in batteries, 3D structural analysis of diffusion layer materials employed in fuel cells and batteries);
- Life science (holotomographic reconstruction of the cellular structure of plants and woods);
- Biology (porosity determination of bone and tooth substance);
- Geology (morphology analysis of minerals);
- Cultural heritage and paleontology (materials characterization).

Synchrotron holo-tomography of insect preserved in Baltic amber



3D Lab - Reference guide for latest publications

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References

[1] Müller, J. *et al.*: Eocene lizard from Germany reveals amphisbaenian origins, Nature 473 (2011), 364-367.

[2] Witzmann, F. *et al.*: Paget disease of bone in a Jurassic dinosaur, Current Biology 21 (2011), R647-R648.

Micro CT | Laboratory for X-ray tomography

TheMicro-CT Lab supports users of the neutron imaging instrument CONRAD-2 and gives the opportunity to perform complementary measurements with X-ray imaging techniques. The micro-spot X-ray source produces a cone beam that allows for a variation of the magnification ratio byadjusting the source-detector and source-sample distances. In this way, the field of view and the spatial resolution are tunable. The short exposure times of a few seconds allow for fast preliminary image tests of samples which are dedicated for neutron tomography experiments.

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Instrument application

- Dynamic radiography
- High-resolution tomography,
- Phase-contrast imaging
- Laminography

Examples

- Energy research (structural investigations of components of Li-ion and alkaline batteries as well as characterization of PEM fuel cell materials);
- Life science (water uptake in plants by using contrast agent and investigation of soil contami nation by heavy metals);
- Biology (investigation of tooth substance and characterization of dental cements);
- Geology (investigation of mineral morphology and crack propagation in rocks);
- Cultural heritage and paleontology (in close col laboration with the local museums).

Typical measuring time

Single images can be taken in a few seconds (0.5 s to 5 s), while tomographic investigations require more than 1000 single projections resulting in measurement times of a few hours.

Parameters

Micro focus X-ray tube	Hamamatsu L8121-3 Voltage: 40 – 150 kV Current: 0-250 µA @ small spot 7 µm 0-500 µA @ middle spot 20 µm 0-500 µA @ large spot 50 µm
Detector	Flat panel (Hamamatsu C7942SK-05) 2316 x 2316 pixels, pixel size: 50 µm Size: 11.5 cm x 11.5 cm
Magnification	Up to 10 times
Best spatial resolution	10 µm at field-of-view 10 mm x 10 mm
Sample manipulator	Rotation table: 0-360° Translation table (along the beam): 60-700 mm Translation table (transverse to the beam): 0-100 mm Maximum weight: 5 kg

References / Latest publications

[1] Müller, J. *et al.*: Eocene lizard from Germany reveals amphisbaenian origins, Nature 473 (2011), 364-367.

[2] Witzmann, F. *et al.*: Paget disease of bone in a Jurassic dinosaur, Current Biology 21 (2011), R647-R648.

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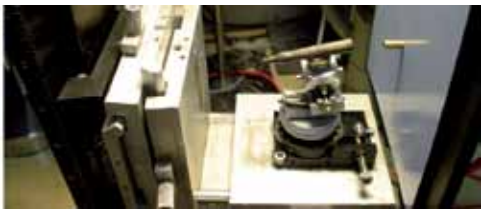
[5] Hautier, L. *et al.*: Skeletal development in sloths and the evolution of mammalian vertebral patterning, Proceedings of the National Academy of Sciences of the USA 107 (2010), 18903-18908.

Micro CT - Reference guide
for latest publications





X-ray Lab – XLab | Laboratory for X-ray experiments

The idea of the X-Lab instruments is to provide X-ray techniques complementary to neutron experiments on one hand, on the other side they are tools for the preparation and characterisation of samples used in neutron scattering and other investigations. To save valuable beam time external users of our facilities are invited to use the superior sample orientation methods and powder characterisation instruments for their experiments at the HZB.

A flexible Laue apparatus is available for single crystal orientation. It can be combined with a precision wire saw and polishing to prepare oriented surfaces with high accuracy. Further, the X-ray suite comprises two powder diffractometers and a four circle single crystal diffractometer which covers a wide temperature range.

The instruments are accessible for HZB scientists as well as for visiting scientists at the HZB under the “calendar of scheduled experiments”. Users will be trained by the staff of the magnetism groups to be able to conduct experiments independently. Please contact the X-Lab responsible or any of the magnetism group staff members.

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X-ray Lab - XLab - Reference guide for latest publications

MX BioLab

The HZB-BioLab at Adlershof is located attached to the BESSY II experimental hall near the cargo port. It is operated by the MX-group to support external and internal users of the HZB for preparing their biological samples (safety level S1).

In addition, it serves as the basis for the expression and purification of recombinant proteins suitable for crystallisation experiments.

The BioLab was completely remodelled in spring 2011. It consists of three separate rooms with different functionalities: sample preparation, crystallization, protein purification and cell cultivation.

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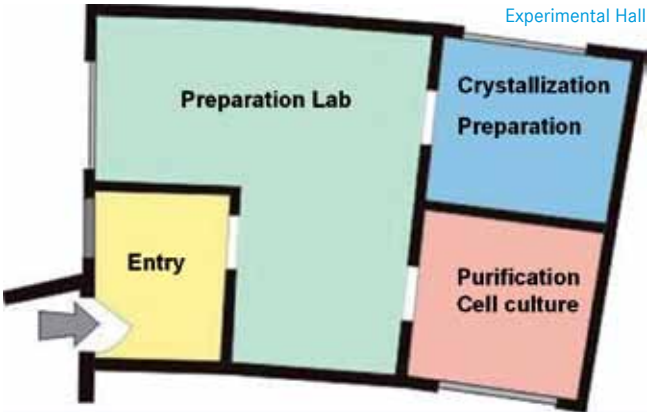
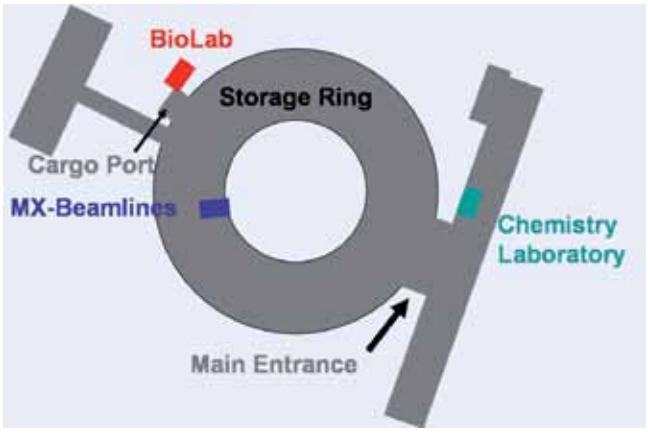


MX BioLab - Reference guide for latest publications



Sputter Lab

The sputtering lab is equipped with a magnetron sputtering system named MAGGSY. Various materials are available to be use by the HZB users for thin film deposition and for sample coating. The parameters of the system are summarized below:

Typical base pressure: $2 \cdot 10^{-8}$ mbar
Partial Ar pressure: $1.5 \cdot 10^{-3}$ mbar
Materials: metals, oxides
Substrates: Si, oxides
Deposition rates: ~0.01-0.1 nm/s
Typical layer thicknesses: 0.1-10 nm

The sample characterization in the sputtering lab is temporarly limited, but possible in the other available HZB user labs. For scheduling you sample growth, please contact the lab responsible at least 5 months in advance of your experiments.

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Sputter Lab - Reference guide for latest publications

HZB Helmholtz Zentrum Berlin

Glossary

BESSY II instrument names

The names of the BESSY II beamlines consist in the name of the insertion device with the number being the length of one magnetic period in the device in mm, *e.g.* **U49. U** stands for undulator (soft X-rays, linear polarized light). For elliptically polarized undulator (soft X-rays, full control over polarization) it is **UE**. For hard X-rays HZB provides wave length shifter (**WLS**) or multipole wiggler (**MPW**), *e.g.* **7T-MPW**. The number indicated the magnetic field of the device in Tesla.

Information on the type of monochromator is added with a counting number in case there is more than one beamline of the same type, *e.g.* **UE56/1-ZPM** (elliptical polarized undulator, 56 mm period length, beamline equipped with a zone plate monochromator (**ZPM**)) or **UE56/2-PGM-2** (second elliptical polarized undulator, 56 mm period length, beamline equipped with a plane grating monochromator (**PGM**))

If there is no insertion device given, the beamline is a dipole-beamline and described only by the monochromator, *e.g.* **PM3** (plate monochromator number 3), **KMC-1** (Kristall-monochromator number 1) or **HE SGM** (high energy spherical grating monochromator (**SGM**))

BER II instrument names

The names at the BER II beamlines consist of the name of the guide hall, **E** for experimental hall, **V** for Versuchshalle, and a counting number of the number of instruments in the hall starting with the oldest instrument, *e.g.* **E1** (experimental hall instrument number 1) or **V7** (Versuchshalle (neutron guide hall) instrument number 7).

Abbreviations

ALD	Atomic layer deposition
APD	Avalanche photodiode
ARPES	Angle resolved photoelectron spectroscopy
ARTOF	Angular resolved time-of-flight
ASAM	Analytical spectroscopy and microscopy
ASAXS	Anomalous small angle X-ray scattering
BAM	Bundesanstalt für Materialforschung und -prüfung
BER II	Berliner Experimentier Reaktor II
BESSY II	Berliner Elektronenspeicherring für Synchrotronstrahlung II
BTU	Brandenburgische Technische Universität Cottbus - Senftenberg
CCD	Charge coupled device
COLTRIMS	Cold target recoil ion momentum spectroscopy
CONRAD	Cold neutron radiography
CRG	Collaborative research group
CSR	Coherent synchrotron radiation
CT	Computer tomography
CXS	Coherent X-ray scattering
DCM	Double crystal monochromator
DLS	Dynamic light scattering
EDDI	Energy dispersive diffraction
EMIL	Energy Materials In-situ Laboratory Berlin
EPR	Electron paramagnetic resonance
EXAFS	Extended X-ray absorption fine structure
EXED	Extreme environment diffractometer
FALCON	Fast acquisition Laue camera for neutrons
FEL	Free electron laser
FIREPOD	Fine resolution powder diffractometer
FZJ	Forschungszentrum Jülich
GID	Grazing incidence diffraction
GISAXS	Grazing incidence small angel X-ray scattering
HE SGM	High energy spherical grating monochromator
HFM	High field magnet
HIKE	High Kinetic Energy Photoelectron Spectroscopy
HAXPES	Hard X-ray Photoelectron Spectroscopy
ICD	Inter-atomic Coulombic decay
IR	Infrared

Abbreviations continued

IRIS	Infrared intense synchrotron radiation
ISISS	Innovative station for *in-situ* spectroscopy
KIT	Karlsruhe Institute of Technology
KMC	Kristallmonochromator
LaMMB	Laboratory for magnetic measurements
LEED	Low energy electron diffraction
LEEM	Low energy electron microscopy
LMC	Lise-Meitner Campus
MAD	Multi-wavelength anomalous diffraction
MAXYMUS	Magnetic X-ray micro- and UHV spectroscope
MCP	Microchannel plate detector
MOKE	Magneto optic Kerr effect
MPG	Max Planck Gesellschaft
MPW	Multipole Wiggler
MX	Macromolecular X-ray crystallography
NEXAFS	Near edge X-ray absorption fine structure
NIM	Normal incidence monochromator
NRSE	Neutron resonance spin echo
PDI	Paul Drude Institut
PED	Photoelectron diffraction
PEEM	Photoemission electron microscopy
PES	Photoelectron spectroscopy
PGM	Plane grating monochromator
PHOENEXS	Photoemission and near edge X-ray station
PM	Plate monochromator
PONTO	Polarized neutron tomography
PTB	Physikalisch Technische Bundesanstalt
RGL	Russian German beamline
RICXS	RIXS/CXS (resonant inelastic x-ray scattering/coherent x-ray scattering)
RIXS	Resonant inelastic X-ray scattering
RSXD	Resonant soft X-ray diffraction
RSXS	Resonant soft X-ray scattering
SAD	Single wavelength anomalous diffraction
SAMIC	Spectroscopy and microscopy integrating chamber
SANS	Small angle neutron scattering
SAXS	Small angle X-ray scattering
SGM	Spherical grating monochromator
SISSY	Solar energy materials *in-situ* spectroscopy at the synchrotron

SMART	Spectro-microscope with aberration correction for many relevant techniques
STXM	Scanning transmission X-ray microscopy
SXPS	Soft X-ray photoemission spectroscopy
TEM	Transmission electron microscopy
THz	Terahertz
TOF	Time-of-flight
TXM	Transmission X-ray microscopy
TXRF	Total reflection X-ray fluorescence
TUD	Technische Universität Darmstadt
UHV	Ultra high vacuum
UPS	Ultraviolet photoelectron spectroscopy
USANS	Ultra small angel neutron scattering
UXRD	Ultrafast X-ray diffraction
WAXS	Wide angle X-ray scattering
WCRC	Wilhelm-Conrad-Röntgen Campus
XAS	X-ray absorption spectroscopy
XANES	X-ray absorption near edge structure
XES	X-ray emission spectroscopy
XM	X-ray microscopy
XMLD	X-ray magnetic linear dichroism
XMCD	X-ray magnetic circular dichroism
XPEEM	X-ray photoemission electron microscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
XRF	X-ray fluorescence
XRS	X-ray reflection spectroscopy
XUV	Extreme ultra violet radiation
ZPM	Zone plate monochromator
XPP	X-ray pump probe

Imprint

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Map
At the HZB-Wannsee site is the Lise-Meitner-Campus with the research neutron source BER II, at HZB-Adlershof the Wilhelm-Conrad-Röntgen-Campus with the electron storage ring BESSY II.