Task 4.6 Development of a generic CDR for automated XAS Beamlines

Melanie Nentwich
Darmstadt, 09.02.2023

Overview

- > Task 4.6 within CREMLINplus
- > Current Status
- > Future Perspectives

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Task 4.6 within CREMLINplus

Task 4.6 within CREMLINplus

- WP4 Collaboration with USSR
- Task 4.6 Scientific case, beamlines and experimental stations: definition of perspective techniques for a 4th generation source
- D4.1 Report on the scientific case and the conceptual design of a **scattering/diffraction** beamline
  due in January 2021
- D4.7 and M24 Report on the scientific case and the conceptual development of a prototype **spectroscopy** beamline
  due in January 2022
- D4.14 and M48 Report on the scientific case and conceptual development of beamlines and experimental stations
  due in January 2024

eurizon
European network
for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a scattering/diffraction beamline

Comparison of nanoprobe beamlines

- from existing and planned 4th generation synchrotron rings 4GSR
- comparing main components and distances

Table 1: Overview of the distances of beam shaping elements at different nanoprobe beamlines of 4GSR.

	ID16B, ESRF-EBS	ID01, ESRF-EBS	NanoMAX, MAX IV	ISN-ID19, APS-U	3DMN-34ID, APS-U	CHEX-28ID, APS-U
aperture	30	–	–	27	27	27
mirrors	30	–	25	29	30	26 + 34
aperture	–	–	–	30	47	–
mono	35	33	28	32	54	35
focusing	–	–	–	35	–	50
SSA	40	100	51	55 + 64	–	50
aperture	164	–	–	–	–	–
focusing	165	119	84/94	220	65	63

eurizon European network for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a scattering/diffraction beamline

Table 2: Beamline parameters of existing nanoprobe beamlines of 4GSR. DCM – double crystal monochromator, CCM – channel cut monochromator, KB mirrors – Kirkpatrick-Baez mirrors, FZP – Fresnel zone plates, CRL – compound refractive lenses, NF – nanofocusing, WBM – white beam mirror, H – horizontal, V – vertical

parameter	unit	ID16B, ESRF-EBS [18]	ID01, ESRF-EBS [19, 20]	NanoMAX, MAX IV [21, 22]	ISN-19ID, APS-U [23, 24]	3DMN-34ID, APS-U [23, 24]	CHEX-28ID, B, APS-U [23, 24]	new beamline for USSR
Ring								
electron beam energy	(GeV)	6.037	6.037	3	6	6	6	6
electron beam current	(A)	0.2	0.2	0.25	0.2	0.2	0.2	0.1
dist. to sample	(m)	165	118	94	67	65	220	100
Undulator								
undulator type		in-vacuum	revolver	in-vacuum	revolver	planar	planar	in-vac.
undulator length	(m)	2.5	1.6	1.5	4.6	2.1	1.3	4
period	(mm)	26	27/35	18	21/25	28	19	23
k value		N/A	N/A	1.95	$K_y = 1.94$	2.46	2.29	2.12
minimal gap	(mm)	6.5	11	4.0	N/A	N/A	N/A	6
energy range	(keV)	5 ... 70	6 ... 24	5 ... 30	5 ... 30	5 ... 30	15 ... 60	5 ... 40
Monochromator								
optical elements		double WBM	–	H & V focusing mirrors	–	flat H mirror	collimators	–
monochromator		V diffracting DCM, Si(111)	CCM & DCM, Si(111)	H diffracting DCM, Si(111)	H deflecting DCM, Si(111)	DCM	H DCM	DCM, Si(111)
offset	(mm)	12.5	N/A	13.3	N/A	1.1	N/A	10.0
End Station								
secondary focusing		KB mirrors	FZP	KB mirrors or FZP	NF mirrors	KB mirrors	CRL	CRL or mirrors
min. beam size	(nm)	50	35	KB: 300, FZP: 40	N/A	37	800	50
flux	(ph/s)	1×10^{12a}	1×10^{9b}	1×10^{12c}	5×10^{12c}	N/A	4×10^{13c}	3×10^{13d}

[a] 17.5 keV, [b] 8 keV, [c] 10 keV, [d] 20 keV

eurizon
European network
for developing new horizons for RIs

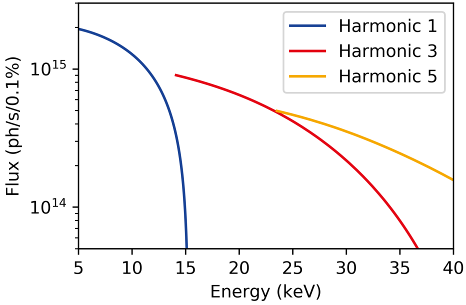
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a scattering/diffraction beamline

Choosing an appropriate undulator

- $5\,\text{keV}$ to $40\,\text{keV}$
- nanoprobe $\rightarrow$ highest brilliance
- available straight section: $5\,\text{m}$
- in-vacuum undulator, effective length of $4\,\text{m}$
- design recommended by M. Tischer, DESY:
  - min. gap: $6\,\text{mm}$
  - magnetic field: $0.987\,\text{T}$
  - period length: $23\,\text{mm}$
  - periods: 174
  - k-value: 2.12

X-Ray Tracing calculations of the undulator



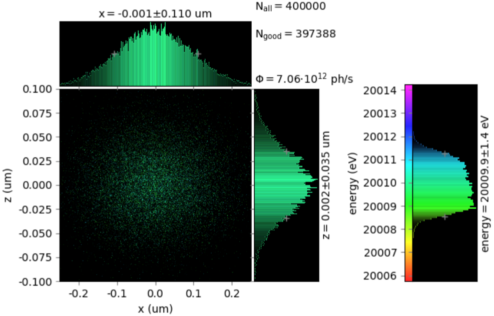
eurizon
European network
for developing new horizons for RIs
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a scattering/diffraction beamline

Choosing focusing elements

- Compound Refractive Lenses (CRL), Fresnel Zone Plates (FZP) or Kirkpatrick Baez (KB) mirrors?
- here: CRLs
  simple handling, “rare” energy changes
- 2D Be lenses, radius 0.05 mm
- large working distance of 0.6 m for extensive sample environments
- optionally combined with a secondary source CRL (SSA at 77 m)

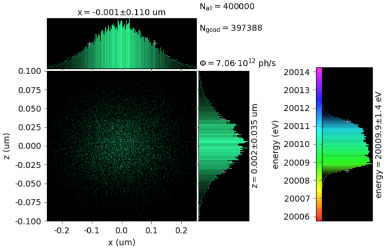
X-Ray Tracing calculations of the CRLs



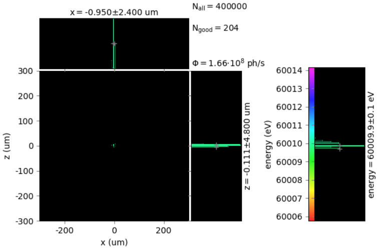
1 set of CRL, $E = 20$ keV, sample position

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

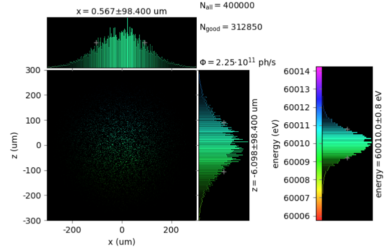
CDR of a scattering/diffraction beamline



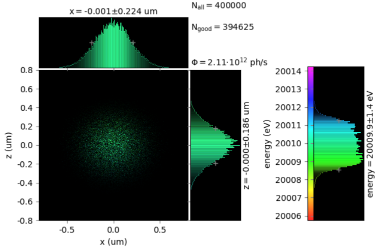
1 set of CRL, $E = 20$ keV, 0.22×0.07 µm^2



1 set of CRL, $E = 60$ keV, pinhole, 4.8×4.8 µm^2



1 set of CRL, $E = 60$ keV, 197×197 µm^2



2 sets of CRL, $E = 20$ keV, 0.45×0.37 µm^2

eurizon
European network
for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a prototype spectroscopy beamline

Comparison of spectroscopy beamlines

- from existing and planned 4th generation synchrotron rings 4GSR
- comparing main components and distances

		Polar 4-ID B [27]	XPCS 8-ID E [27]	Balder[a] [28, 29]	ID24 EDXAS_L [30]	ID26, EH1 [31, 32]
	aperture	27.0	27.1	–	N/A	–
	WBM/HRM	2×28.5	$28.0 + 30.6$	$26.5 + 31.5$	$28.5 + 31.0$	29.7
	monochromator	30.0	33.7	28.0	55.0[b]	33.4
	aperture	31.1	–	31.0	N/A	34.2
	aperture	47.3	51.3	–	N/A	–
focusing	toroid mirrors	$48.0 + 50.0$	–	31.5	55.5	–
focusing	KB mirrors	61.0	55.3	–	$28.5 + 31.0$	$37.2 + 39.1$
focusing	transfocators	59.3	52.0	–	–	–
	attenuators	54.1	N/A	N/A	N/A	41.9
	aperture	53.7	54.8	32.0	N/A	42.0
	aperture	59.4	55.9	–	N/A	–
	sample	61.3	56.3	46.0	55.6	43.0

eurizon
European network
for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a prototype spectroscopy beamline

Comparison of spectroscopy beamlines

- from existing and planned 4th generation synchrotron rings 4GSR
- comparing main components and distances

		EMA [33, 34]	QUATI [35]	P64 [36, 37]	P65 [38]
	aperture	N/A	N/A	44.8 + 37.1	49.0
	WBM/HRM	2×33.3^c	15.0 + 30.0	58.7 + 60.1	50.0 + 53.0
	monochromator	28.5	24	56.6	51.5
	aperture	N/A	N/A	–	–
	aperture	N/A	N/A	–	–
focusing	toroid mirrors	–	30	–	–
focusing	KB mirrors	44.5 + 96.0	–	–	–
focusing	transfocators	–	–	–	–
	attenuators	45, 97	N/A	N/A	N/A
	aperture	–	N/A	87	59
	aperture	–	–	–	N/A
	sample	98	45	87.2	60

eurizon European network for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a prototype spectroscopy beamline

parameter	unit	Polar 4-ID, APS-U [27]	XPCS 8-ID, APS-U [27]	Balder, MAX IV [28, 29]	ID24 EDXAS_L, EBS-ESRF [30]	ID26, EBS-ESRF [31, 32]
Ring						
electron beam energy	(GeV)	6	6	3	6.037	6.037
electron beam current	(A)	0.2	0.2	0.25	0.2	0.2
Undulator						
undulator type		2 in-line SCAPE[a]	2 in-line revolver	in-vacuum, tapered	4 in-line, 'tapered'	3 in-line
undulator length	(m)	2×1.3	4.6	2.0	$\approx 3 \times 1.5$	3×1.6
period	(mm)	$35 + 35$	21/25	50	$27 + 27 + 27/32 + 32$	$35 + 35 + 35$
k value		N/A	1.29/1.90	9	N/A	2.45
minimal gap	(mm)	N/A	N/A	5.5	*e. g.* 11.0/11.7/12.5	11.2
energy range	(keV)	2.8 to 27	8 to 25	2.4 to 40	5 to 28	2 to 25
Monochromator						
optical elements		WBM (Si, Pt, Rh)	WBM (Si, Cr, Pt, Rh)	WBM (Si, Ir)	KB-V = WBM (Si, Pt, Rh)	WBM (Si, Pt, Pd)
monochromator		H DCM, Si(111), LN_2 cooled	H DCM, Si(111) and Si(113), LN_2 cooled	DCM, Si(111) and Si(113), LN_2 cooled	polychromator, Si(111), Laue geometry	DCM, Si(111) and Si(113), LN_2 cooled
offset	(mm)	N/A	15	10 to 32	N/A	25
End Station						
no. end stations		2	2	1	2	2
dist. source to sample	(m)	61.3/73.3	56.3/67.5	46.0	55.6/64.7	43.0/54.6
focusing elements		transfocators, KB mirrors, toroidal mirrors	transfocators, KB mirrors	toroidal mirror	KB mirrors	bendable KB mirrors
beam size	(μm^2)	34×4	0.3×0.3	100×100	4×4	100×50
flux	(ph/s)	N/A	N/A	1×10^{13}[b]	4×10^{13}[c]	5×10^{13}[d]
diffractometer		double tilt Eulerian cradle	double tilt Eulerian cradle	1 axis	breadboard	breadboard
detectors etc.		2D fluorescence D, polarization A, Raman S	N/A	Raman S, mass S, X-ray emission S, Lytle D, PIPS D, SDD	2D FReLoN CCD, 1D Hamamatsu CCD, XH Ge microstrip	photo diodes, hard X-ray emission S, tender X-ray emission S, SDD

uperConducting Arbitrarily Polarizing Emitter, *b* – over complete energy range, *c* – 24 keV, *d* – no details given

eurizon
European network
for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

CDR of a prototype spectroscopy beamline

parameter	unit	EMA, Sirius [33, 34]	QUATI, Sirius [35]	P64, PETRA III [36, 37]	P65, PETRA III [38]	new beamline for USSR
Ring						
electron beam energy	(GeV)	3	3	6	6	6
electron beam current	(A)	0.1	0.1	0.1	0.1	0.2
Undulator						
undulator type		in-vacuum	dipole source	??	mini-undulator	revolver
undulator length	(m)	1.2	N/A	2	0.39	4
period	(mm)	20	N/A	32.8	32.8	27
k value		N/A	N/A	2.7	2.6	2.12
minimal gap	(mm)	22	N/A	9.5	10	6
energy range	(keV)	2.7 to 30	4.5 to 35	4 to 44	4 to 44	4 to 39
Monochromator						
optical elements		HRM (Si, Pt, Rh)	WBM (Si, Pt, Rh)	WBM (Si, Pt, Rh)	WBM (Si, Pt, Rh)	–
monochromator		DCM, Si(111) and Si(220), V bounce, fixed exit	DCM, Si(111) and Si(311), LN_2 cooled	CCM and DCM, Si(111), Si(311), LN_2 cooled	DCM, Si(111) and Si(311), H_2O cooled	
offset	(mm)	0	N/A	21	N/A	0
End Station						
no. end stations		2	2	1	1	
dist. source to sample	(m)	45.5/98	45.5	87.2	N/A	70?
focusing elements		KB mirrors	toroidal mirror (Pt, Rh)	mirrors (Si, Rh)	–	
beam size	(μm^2)	1×0.4	10×5	150×50	500×1000	0
flux	(ph/s)	1×10^{12e}	1×10^{10e}	1×10^{13f}	2×10^{12f}	5×10^{13g}
diffractometer		6+2 circles	breadboard	breadboard	breadboard	??
detectors etc.		2D, Raman-S, photodiodes, ion chamber, fluo D	Raman-S	fluorescence D, transmission D, ion chamber, dispersive von-Hamos S	ion chamber, HPGe D, Si-PIPS^h diodes, fluo D	

e – 20 keV, f – 9 keV, g – experimental values, h – Passivated Implanted Planar Silicon

eurizon European network for developing new horizons for RIs

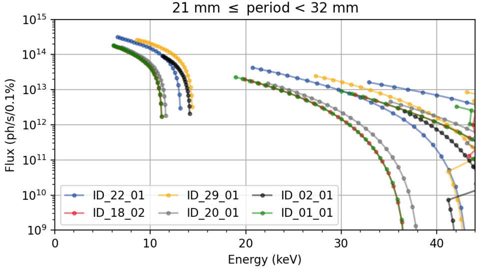
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

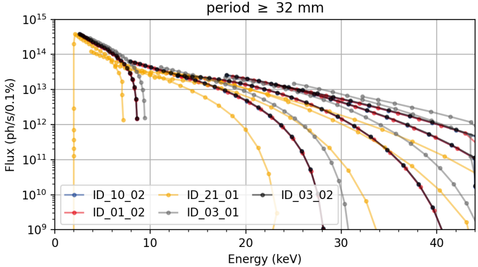
CDR of a prototype spectroscopy beamline

Choosing an appropriate undulator

- $5\,\text{keV}$ to $40\,\text{keV}$
- highest brilliance $\rightarrow$ penetrate sample environments AND minimize exposure time (increase time resolution)
- using well established ESRF design (55 models listed)
- complementing revolver, in-air undulators, effective length of $2.5\,\text{m}$
  - analyzing groups of undulators with period below and above $32\,\text{mm}$
  - U23 (ID 22_01)
  - U35 (ID 03_02)

X-Ray Tracing calculations





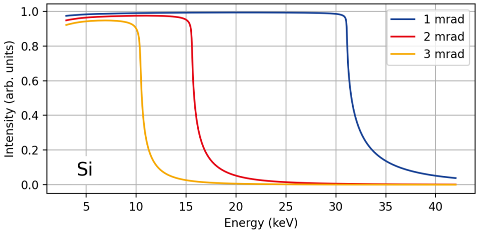
eurizon European network for developing new horizons for RIs
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

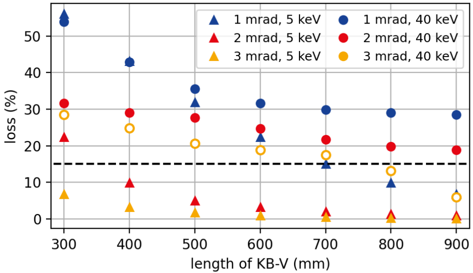
CDR of a prototype spectroscopy beamline

Choosing optical elements

- avoid energy dependent monochromator offset: 2 sets of channel-cut monochromators
  additional benefit: sharpening of beam profile while almost no additional loss of intensity
- focusing with KB mirrors (non-dispersive)
  - Si with Rh and Pt coating
  - determining KB size (minimizing cutting-off the beam): 500×30 mm and 400×30 mm

X-Ray Tracing calculations





eurizon European network for developing new horizons for RIs
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Current Status

Changes towards EURIZON

- WP4 Synchrotrons
- Task 4.6 Development of a generic Conceptual Design Report for automated X-Ray Absorption Spectroscopy Beamlines
- D4.22 Report on the 1st International Workshop due in January 2023
- M59 Input collection finalized due in June 2023
- D4.23 Completion of the generic **CDR for a fully automated XAS beamline** due in December 2023
- D4.24 Report on the 2nd International Workshop due in January 2024

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Current progress within EURIZON

- > Oct. 2022:
  - starting to organize the workshop
  - cooperation with managers of XAS beamlines at DESY
  - dedicated session within the XAS satellite workshop at the DESY Users' Meeting (23 – 27 January 2023)
- > Nov. 2022: gaining overview of relevant aspects (automation, XAS, in-situ, …)
- > Dec. 2022: choosing topics and inviting speakers
- > Jan. 2023: performing workshop including 6 speakers and more than 70 participants online and in-person

SATELLITE WORKSHOP - Photon Science

DESY.

X-Ray Absorption Spectroscopy today and perspectives for future PETRA III and IV beamlines

Thursday, 26. January 2023 , Bldg.3 BAH I + II

Organizers: W. Caliebe, E. Welter, M. Nentwich (DESY)

PROGRAMME

	Beamline Automation	
14:45	Automatization of synchrotron experiments - present and future	Alexander Schökel
15:05	SECoP - the Sample Environment Communication Protocol	Klaus Kiefer (Via Zoom)
15:25	TBD	Peter Weidler
15:45	XAS reference database under DAPHNE4NFDI	Sebastian Paripsa
16:05	Relevanz von Automatisierung in der Industrie	Bernd Hinrichsen
16:25	TBD	Janis Timoshenko
16:45	Discussion	
17:00	**End of Meeting**	

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Future Perspectives

Future Perspectives

- evaluation of 1st workshop
- identifying critical topics and issues
- detailed investigations (M59, due in June 2023)
- performing xrt calculations to beamline details (yet to be defined)
- writing CDR (D4.23, due in December 2023)
- preparing the 2nd workshop (presenting CDR)
- report on 2nd workshop (D4.24, due in January 2024)

eurizon European network for developing new horizons for RIs

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Conclusion

- CDR for nanobeam diffraction/scattering beamline
  - comprehensive comparison of existing/ planned beamlines at 4GSR
  - including xrt model of the beamline for adaption
- CDR for prototype spectroscopy beamline
  - comprehensive comparison of existing/ planned beamlines at 4GSR
  - detailed calculations on the design of the KB mirrors
  - including xrt model of the beamline for adaption
- 1st workshop was held successfully

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

Thanks to

EURIZON
for financial support

DESY
Oliver Seeck
Dmitri V. Novikov

ESRF
Michael Krisch

You
for your attention

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.