Approaches to the design of second-phase SKIF beamlines

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Synchrotron and free-electron laser radiation: generation & application 16.07.2020

SRF “SKIF” RESEARCH INFRASTRUCTURE

- 30 beamlines in total
- 14 beamlines use SR of IDs installed in straight sections (11 undulators & 3 wigglers)
- 8 beamlines use high-field BMs (2.05 T)
- 8 beamlines use low-field BMs (0.52 T)
- 4 undulator and 2 wiggler beamlines at the 1st phase
- 2nd phase: 8 IDs, 8 HF-BMs, 8 LF-BMs

ПРАВИТЕЛЬСТВО РОССИЙСКОЙ ФЕДЕРАЦИИ

ПОСТАНОВЛЕНИЕ
от 16 марта 2020 г. N 287

ОБ УТВЕРЖДЕНИИ ФЕДЕРАЛЬНОЙ НАУЧНО-ТЕХНИЧЕСКОЙ ПРОГРАММЫ РАЗВИТИЯ СИНХРОТРОННЫХ И НЕЙТРОННЫХ ИССЛЕДОВАНИЙ И ИССЛЕДОВАТЕЛЬСКОЙ ИНФРАСТРУКТУРЫ НА 2019 - 2027 ГОДЫ

В целях реализации Указа Президента Российской Федерации от 25 июля 2019 г. N 356 "О мерах по развитию синхротронных и нейтронных исследований и исследовательской инфраструктуры в Российской Федерации" Правительство Российской Федерации постановляет:

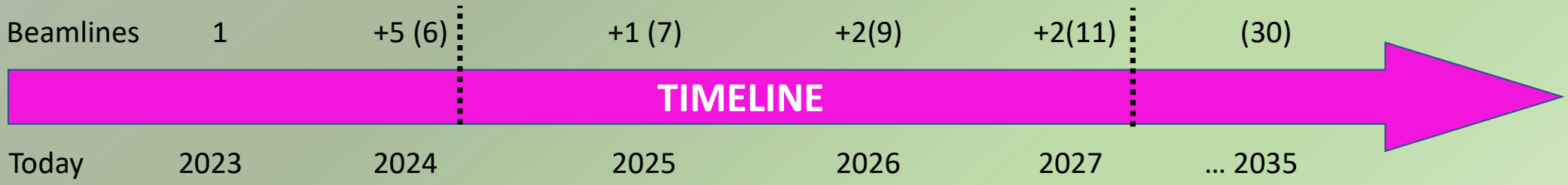
1. Утвердить прилагаемую Федеральную научно-техническую программу развития синхротронных и нейтронных исследований и исследовательской инфраструктуры на 2019 - 2027 годы.

2. Министерству науки и высшего образования Российской Федерации в 6-месячный срок со дня вступления в силу настоящего постановления обеспечить принятие нормативных правовых актов, необходимых для реализации Программы, утвержденной настоящим постановлением.

3. Министерству науки и высшего образования Российской Федерации совместно с заинтересованными федеральными органами исполнительной власти и федеральным государственным бюджетным учреждением "Национальный исследовательский центр "Курчатовский институт" представлять в Правительство Российской Федерации ежегодно, начиная с 2021 года, до 25 марта года, следующего за отчетным, проект доклада Президенту Российской Федерации о ходе реализации Программы, утвержденной настоящим постановлением.

4. Настоящее постановление распространяется на правоотношения, возникшие с 25 июля 2019 г.

Председатель Правительства
Российской Федерации
М.МИШУСТИН



2nd phase beamlines

Selection criteria

- Implementation of techniques uncovered by the 1st phase beamlines but highly important and user-demanded for the next decade
- Comprehensive utilization of unique beam characteristics provided by the generation «4+» source
- Non-standard sample preparation and data acquisition conditions (e.g., biologically hazardous and radioactive samples)
- Guarantee of 100% uptime of basic techniques (spare beamtime in the case of technical failures and shutdowns occurring with the 1st phase beamlines)
- Solid background for sustainable instrumental development (both in-house and with external collaboration)

Groups of beamlines: special environment, methodical development, education, international collaboration, uninterrupted operation, technology (instrumental development)

Design of the 2nd phase beamlines will rely on proven most efficient solutions elaborated during construction of the 1st phase beamlines

ID-based 2nd phase beamlines

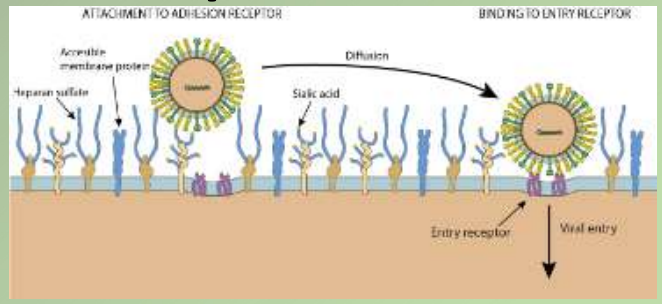
BL Code	Name	Source	Techniques & Energy range	Applications	Features	Group
2-1	Vector	Undulator BLS4U	CDI (1.5-4.0 keV) MX (~12.5 keV) SAXS (~8 keV)	Structural virology, accelerated structure-driven discovery of vaccines and antiviral drugs	Separate building, Biosafety level BSL-3 	Special environment
2-3	NSTU	SC wiggler BLS6W	Diffraction microscopy, PDF, EXAFS 50-80 keV	Construction and engineering materials *operando* (friction & wear, fatigue destruction, welding, laser & plasma surface processing, additive technologies)	Robust design to enable high-throughput measurements by students and promote innovative activity	Education
2-4	Bel-SR	SC Undulator BLS2U	Ptychography, coherent nanoscopy 1.5-4.0 keV	Microelectronics, topology control of 7 nm CPUs	Very long optical scheme (~140 m), diffraction-limited CRL- and μKB-based focusing	International Collaboration (Republic of Belarus)
3-3	Protein	Two canted SC undulators (BLS14U)	High-throughput MX with SAD (2 side branches, 12.5 keV) and MAD (central branch (5-20 keV) phasing, serial crystallography	Structure-driven drug design	Two side branches horizontally bounced via diamond splitters and one central branch equipped with a DCM, highy automated operation	Uninterrupted operation (spare resource for 1-1-3)
3-4	Single Crystal	SC Undulator BLS7U	High-throughput small-molecule crystallography, photocrystallography, perturbation crystallography, 10-30 keV	Basic solid state sciences and development of functional materials	Pump-probe time-resolved experiments using an assortment of HP-HT cells, pulse lasers, etc.	Uninterrupted operation (spare resource for 1-2-3)
3-5	Spectrum	Two canted helical undulators (BLS11U) 0.1-15 keV	X-ray spectroscopies with variable polarization in the soft & tender photon energy ranges at once	Electronic structure and magnetism at the nanoscale	Two independent optical paths for soft and tender X-ray beams focused at the same sample position	Methodical development
3-6	Soft nanoscope	Electromagnetic undulator BLS12U	STXM PEEM 0.1-1.2 keV	Subcellular imaging of bioobjects Microelectronic devices and magnetic memory units	Two independent inline instruments with a common optical scheme	Methodical development
3-7	Gamma-2	SC Undulator BLS11U	Gamma-resonance (Mössbauer) spectroscopy, nuclear inelastic scattering for isotopes other than ^{57}Fe (^{40}K, ^{119}Sn, ^{121}Sb, ^{125}Te, ^{149}Sm, etc.) 10-40 keV	Alloys and intermetallic compounds, HTSC, SOFC, minerals	High-resolution monochromator based on nested back-reflection channel-cuts	Methodical development

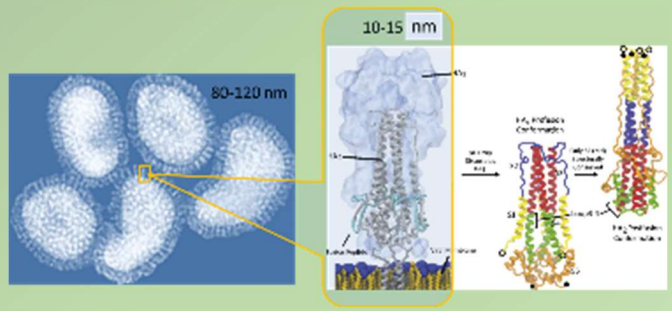
Beamline 2-1 “Vector” (under design in a collaboration with State Research Center of Virology and Biotechnology VECTOR)

Structural virology and accelerated discovery of novel vaccines and antiviral drugs

Problems to be addressed

1. Structure of viral envelope proteins with their relation to the mechanism of attachment to cell adhesion receptors
2. Conformational lability (pH-dependent) of viral envelope proteins and its role in the process of viral entry into a cell
3. Conformational lability of viral envelope proteins and its role for the viral assembly inside the cell and further budding
4. Structure of viral enzymes and search for instruments to control (e.g., inhibit) their activity
5. Glycosylation of viral proteins as a tool to control viral activity





Beamline 2-1 “Vector” (under design in a collaboration with State Research Center of Virology and Biotechnology VECTOR)

Structural virology and accelerated discovery of novel vaccines and antiviral drugs

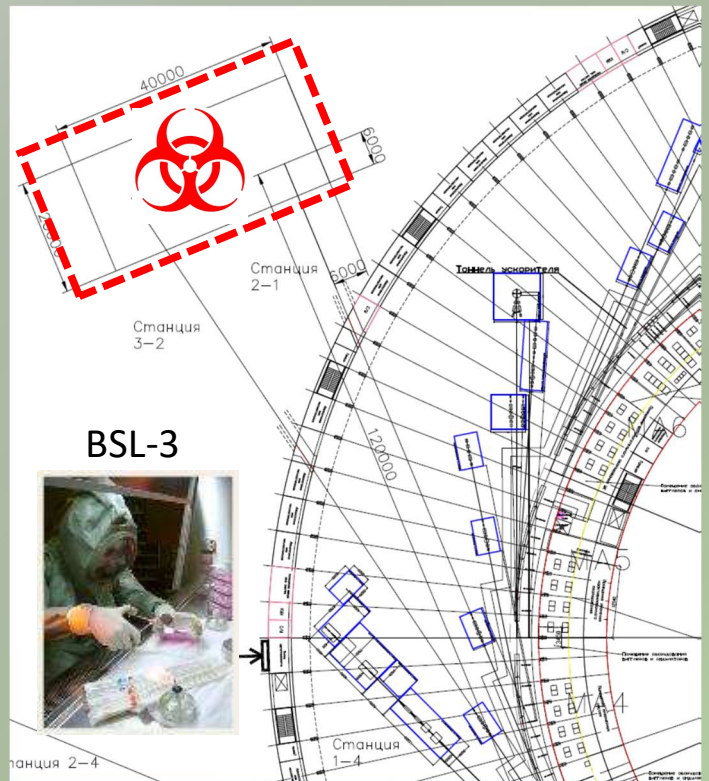
General approach

1. Identification of viruses with ‘pandemic potential’
2. Expression, purification, crystallization of viruses and viral proteins
3. Structure solution of crystals formed by virus particles and viral proteins in an inactive form (SR MX)
4. Characterization of conformational lability of molecular fragments at the surface of active viruses at various stages of their life-cycle (SR CDI)
5. Identification of vulnerability points of viral activity for potential inhibition
6. Structure-driven search for potentially efficient inhibitors (MD and molecular docking simulations). Identification of lead-compounds
7. Combinatory synthesis of predicted virus-inhibitor complexes and solving their structures (SR high-throughput MX & serial crystallography)
8. Tests of inhibition activity on infected cell cultures
9. Elaboration of practical dosage forms and targeted delivery systems for vaccines or antiviral drugs
10. Preclinical studies on therapeutic efficacy with laboratory animals (SR CT)

Beamline 2-1 “Vector” (under design in a collaboration with State Research Center of Virology and Biotechnology VECTOR)

Structural virology and accelerated discovery of novel vaccines and antiviral drugs

Implementation



BSL-3

Coherent diffraction imaging @ 1.5-4.0 keV with an undulator source optimized for increased coherent fraction

Routine and high-throughput macromolecular crystallography @ ~12.5 keV

Serial crystallography for microcrystals

Small-angle X-ray scattering with XPCS and cross-correlation analysis modes

An *ad hoc* plunger injector for water suspensions or aerosols of virus particles

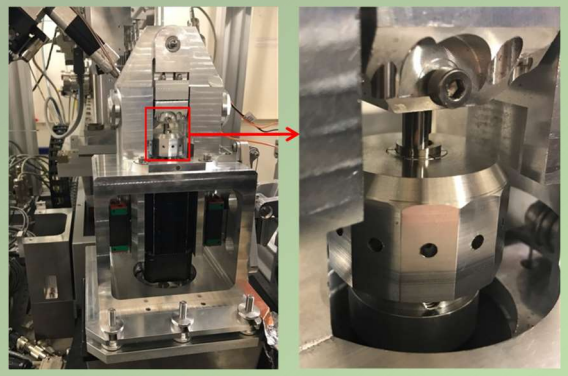
BSL-3 compliant biosafety infrastructure (a separate building with specialized filters, waste treatment, restricted access policies, etc.)

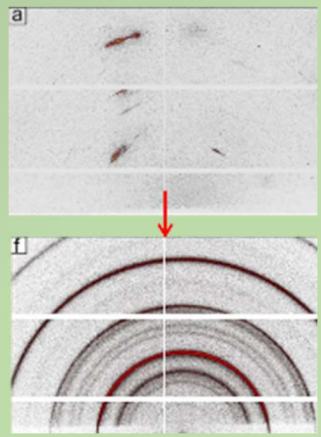
Beamline 2-3 “Novosibirsk State Technical University (NSTU)”

Real-time studies of construction materials during their formation and operation with hard X-ray photons

Processes:

- Sintering
- Mechanical load and deformation
- Friction, aging, corrosion
- Local melting-recrystallization
- Laser and e-beam welding
- Additive technologies and 3D-printing
- Plasma-surface interactions





Materials

- Metals, industrial alloys
- Ceramics
- Biocompatible composites

Techniques

Various types of powder X-ray diffraction, diffraction microscopy, to a limited extent PDF and EXAFS

Photon energy 50-80 keV

Goals:

- The beamline should be seamlessly integrated into the education process
- The beamline should be routinely operated by students during their practice work or thesis preparation (user friendly and safe)
- It should promote innovative activity being able to readily accommodate designed auxiliary equipment for testing

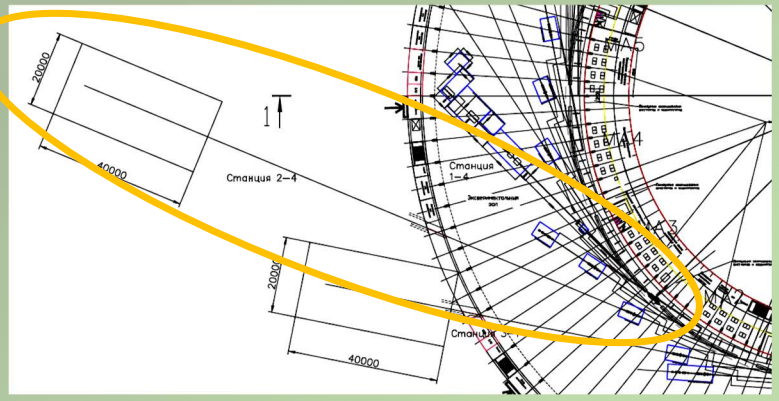
Beamline 2-4 “Bel-SR”
(in a collobaration with National Academy of Sciences of Belarus)

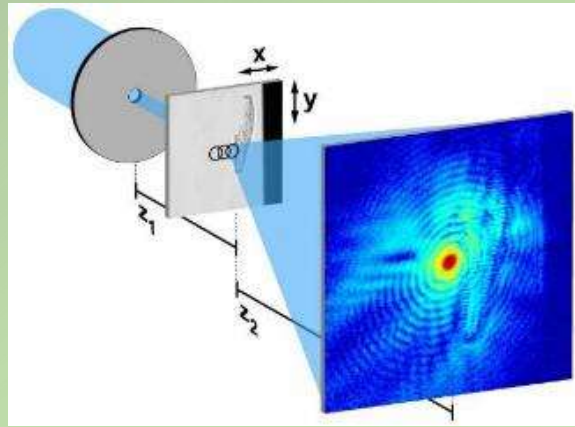
Diagnostics of nanoelectronic devices with coherent X-ray beams at record-high spatial resolution

Total length of optical scheme ~140 m
Diffraction-limited focusing with short-focal-length CRL & μKB mirrors

Techniques: lensless X-ray microscopy, coherent diffraction imaging, ptychography, tomography, X-ray fluorescence 3D-mapping

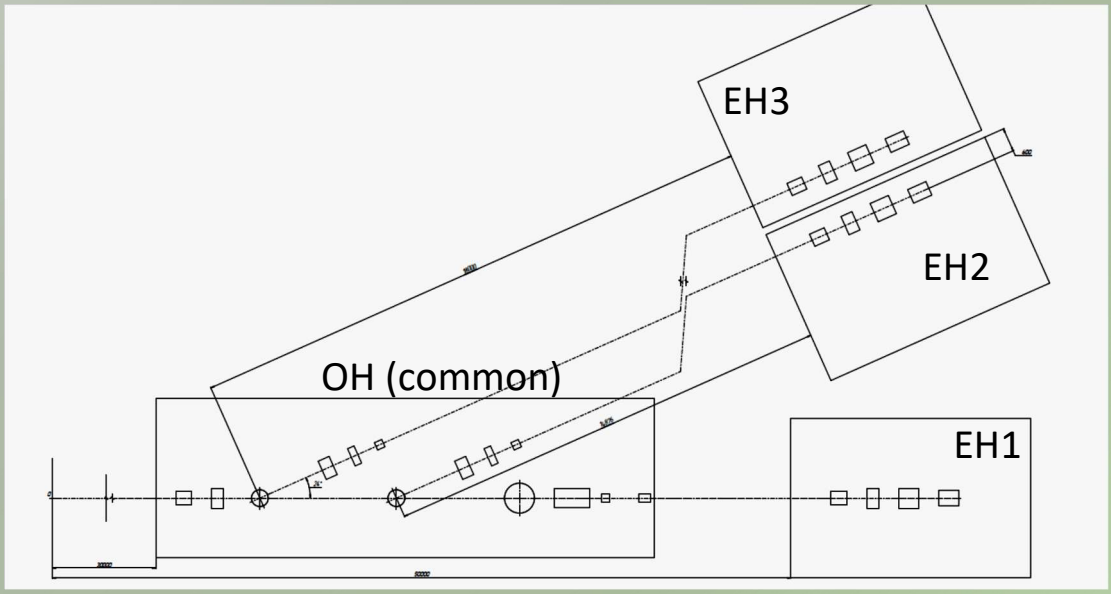
Target spatial resolution: 1 nm

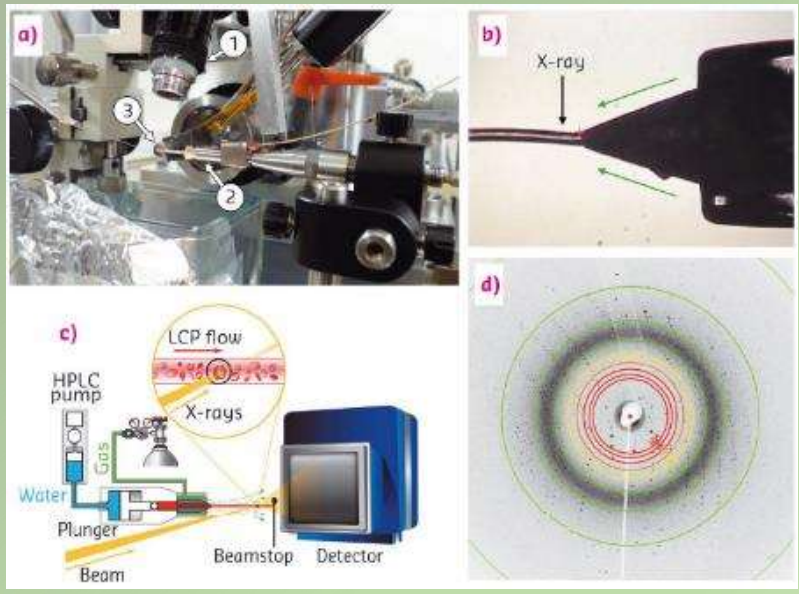


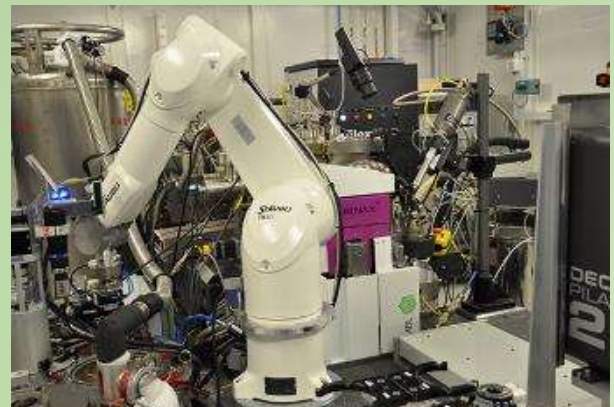


Design similar to NanoMax of MAX IV, Carnaúba of Sirius

Beamline 3-3 “Protein”
Highly automated macromolecular crystallography (including serial crystallography) with MAD phasing option





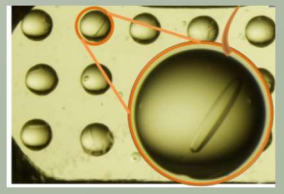


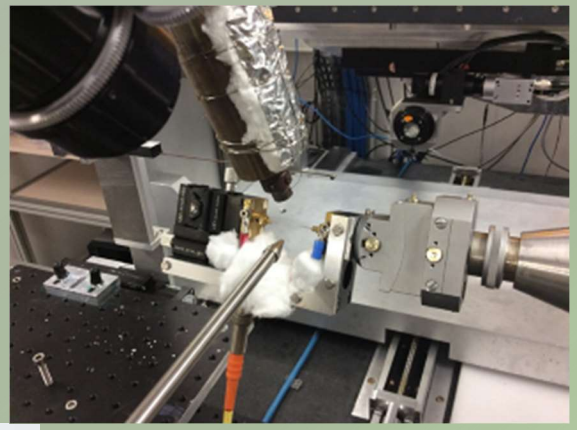
Source: two canted undulators to serve side and central branches
Diamond splitters as monochromators for side branches
DCM for the central branch
Robotic sample changers

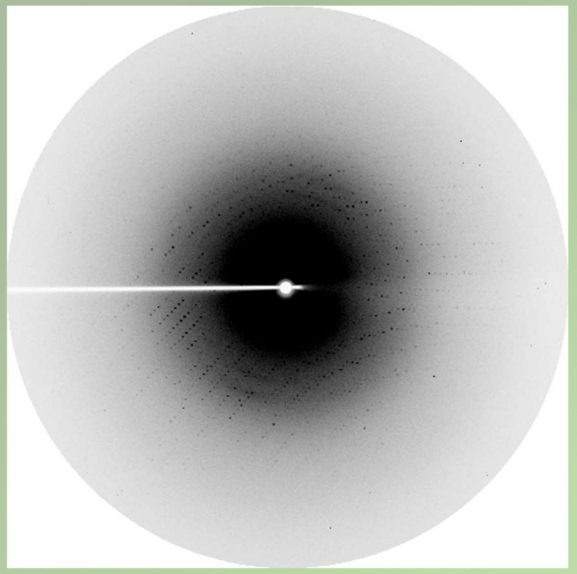
Design similar to MASSIF (ID-30) of ESRF-EBS

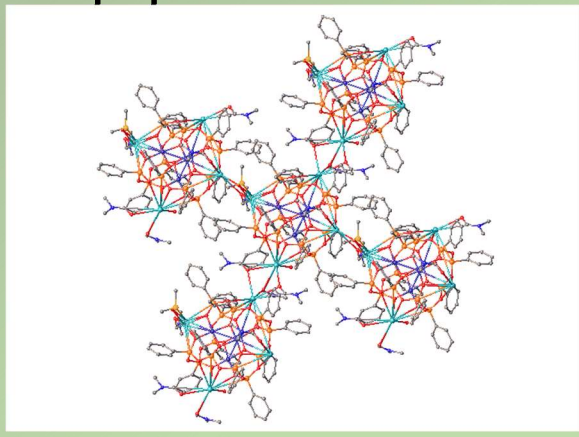
Beamline 3-4 “Single crystal”

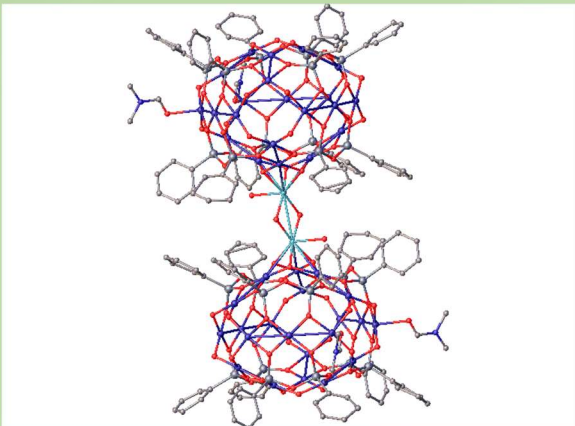
High-throughput small-molecule crystallography. Emphasis on microcrystals, extreme conditions, time resolved and pump-probe experiments











Beamline 3-5 “Spectrum”

Multifunctional X-ray spectrometer operating in soft & tender X-ray ranges

(0.1-15 keV) with variable linear/circular polarization

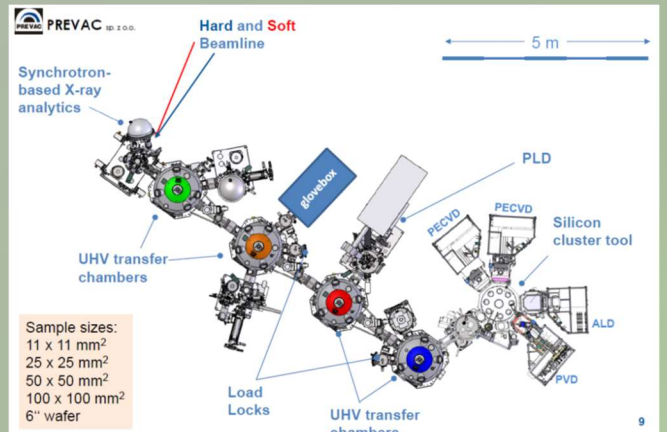
Techniques: XPS/HAXPES, XAFS/XMCD, XES/RIXS

Source: two canted helical undulators generating soft and tender X-ray beams misaligned by ca. 2°

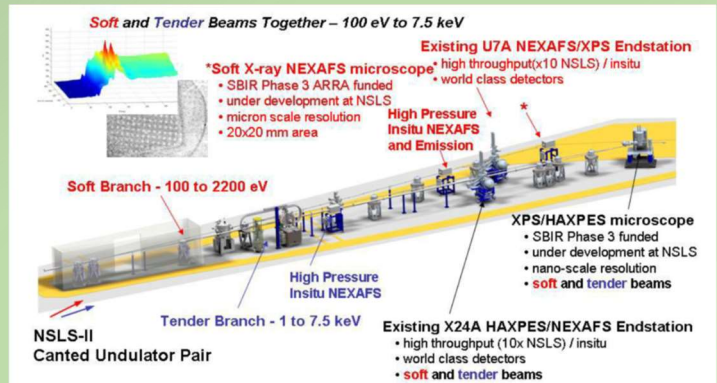
Two independent optical systems guiding the soft and tender beams to a common focal spot on a sample

Design similar to:

EMIL at BESSY II



NIST Soft and Tender X-ray Spectroscopy and Microscopy (SST) beamline at NSLS II



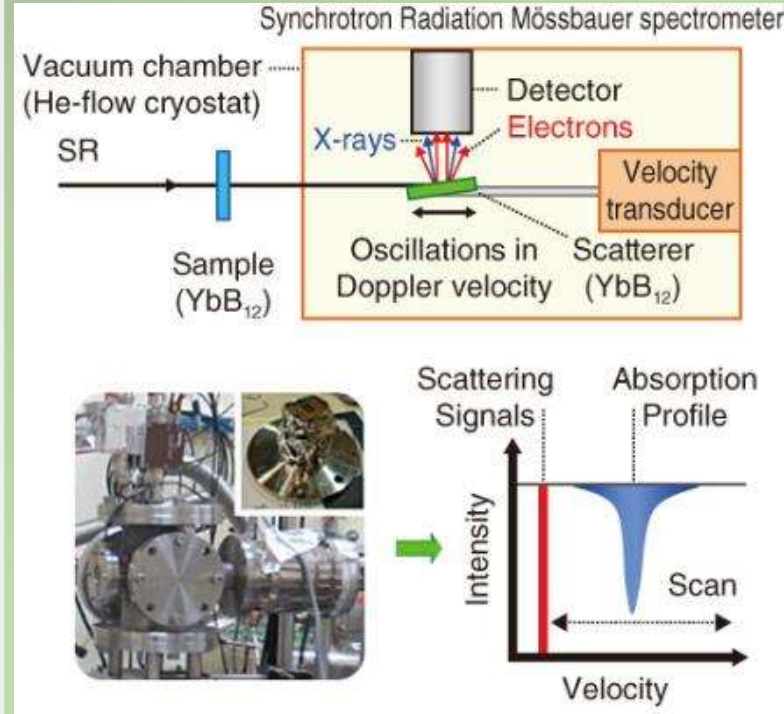
Beamline 3-7 “Gamma-2”
Mössbauer spectroscopy of exotic nuclei (other than ^{57}Fe)

Nested back-scattering channel-cut monochromators for improved energy resolution

Isotope	Energy (keV)	Reflections	Resolution(meV)
^{181}Ta	6.21	Si311-Si511-Si511	10.5
^{57}Fe	14.41	Ge333-Si975-Si975	0.8
	14.41	Si511-Si975(nested)	2.5
	14.41	Si511-Si975(nested)	3.5
^{151}Eu	21.54	Si422-Si12 12 8(nested)	1.7
^{149}Sm	22.51	Si422-Si16 8 8(nested)	1.6
^{119}Sn	23.87	Si440-Si12 12 12(nested)	1.6
^{40}K	29.83	Si660-Si22 14 0	2.6
^{125}Te	35.49	αAl_2O_3 9 1 -10 68	1.7
^{121}Sb	37.13	Si444-Si12 12 8	1.7

Design similar to BL09XU of Spring-8

Nuclides	Natural abundace (%)	Energy (keV)	Half life (ns)
^{40}K	0.0117	29.8299	4.24
^{57}Fe	2.2	14.412497 [23]	98.3
^{61}Ni	1.14	67.413	5.34
^{73}Ge	7.73	68.752	1.74
^{83}Kr	11.5	9.4035 [24]	147
^{99}Ru	12.7	89.68	20.5
^{119}Sn	8.59	23.8795 [25]	18.03
^{121}Sb	57.36	37.133	3.46
^{125}Te	7.139	35.4922	1.48
^{127}I	100	57.608	1.95
^{129}Xe	26.4	39.578	0.97
^{133}Cs	100	80.9974	6.28
^{145}Nd	8.3	72.5	0.72
^{149}Sm	13.8	22.507	7.12
^{151}Eu	47.8	21.54149 [26]	9.6
^{158}Gd	24.84	79.51	2.52
^{161}Dy	18.9	25.6515	29.1
^{168}Er	26.8	79.804	1.88
^{169}Tm	100	8.4103	4.08
^{174}Yb	31.8	76.471	1.79
^{176}Hf	5.206	88.351	1.43
^{181}Ta	99.988	6.214 [27]	6050
^{183}W	14.3	46.4839	0.188
^{189}Os	16.1	36.202	1.62
^{193}Ir	62.7	73.044	6.09
^{197}Au	100	77.351	1.91
^{201}Hg	13.18	32.138	0.1
^{238}U	99.2745	44.91	0.203

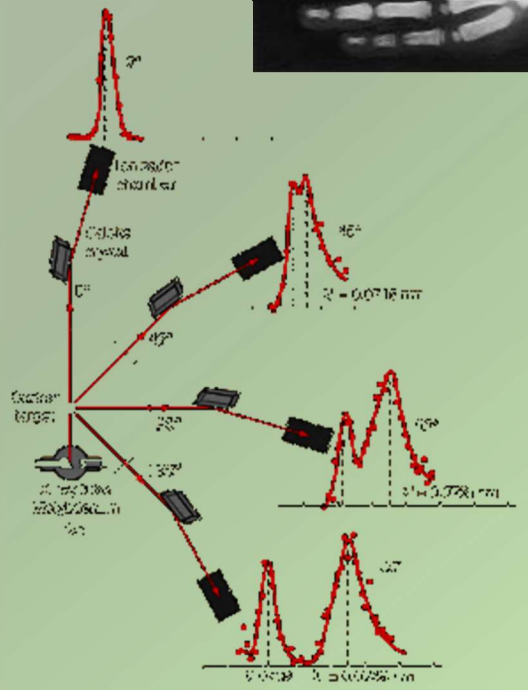


2nd phase beamlines @ HF-BMs

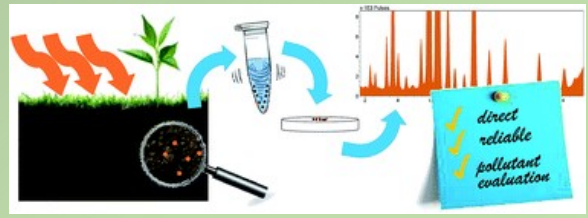
BL Code	Name	Source	Energy range & Techniques	Applications	Features	Group
2-2	NSU	HF-BM	Assortment of X-ray techniques Scattering-Spectroscopy-Imaging in basic configuration 10-40 keV	First familiarization with SR techniques and equipment, history of science, bright visual experiments in biology, physics, materials science	Simple and reliable to design for students, efficient inclusion in educational process	Education
3-1	Isotope	HF-BM BLA1_3H	XRD, EXAFS, SAXS, Fluorescence Analysis, Tomography 10-40 keV	Nuclear medicine and radioecology	Separate building with special security and radioprotection 	Special environment
3-2	Vector Image	HF-BM BLA3_3H	Medicine-oriented high-throughput computed tomography of small and medium-sized mammals with absorption (I-, Ba-, Xe-, or Gd-based contrasting agents) and phase contrast) 30-50 keV	Elaboration of pharmaceutical dosage forms and preclinical tests (vaccines & antiviral drugs)	The same building as 2-1, Biosafety level BSL-3 	Special environment
3-8	SAXS	HF-BM BLA16_3H	Basic SAXS techniques, including ASAXS and GI-SAXS 5-35 keV	Nanomaterials, catalysts, colloids, protein solutions	Assortment of special cells: flow-through capillary, rheology, mechanical deformation	Uninterrupted operation (spare resource for 1-2-4)
3-9	XAFS	HF-BM BLA2_3H	Transmission & Fluorescence yield XAFS 2-35 keV	Catalysts, functional matterials, Li-ion batteries, etc.	Reactive cells for in situ and operando modes	Uninterrupted operation (spare resource for 1-4)
3-10	High-precision X-ray crystallography	HF-BM BLA14_3H	Small-molecule crystallography aimed at reconstruction of electron density maps with multipole refinement and topological analysis within Bader AIM theory 5-35 keV	Fundamental theory of chemical bonding, structure-reactivity correlations	Careful incident intensity control for increased accuracy	Uninterrupted operation (spare resource for 1-2-3)
3-11	Surface	HF-BM BLA4_3H	X-ray reflectivity, GI-XRD, GI-SAXS, Crystal truncation rods 5-35 keV	In situ monitoring of functional film growth	Ion-plasma deposition unit included	Methodical development
3-12	Development (hard X-ray)	HF-BM BLA15_3H	Optical element testing, metrology, feasibility studies of novel concepts 5-35 keV	In-house instrumentation development	Robust and flexible design to meet various requirements	Technology

Beamline 2-1 “Novosibirsk state university (NSU)”

Flexible simple-in-operation education-oriented beamline with an assortment of optical and detecting equipment to setup various experiments in diverse scientific fields



Physics: radiation interaction with matter
Chemistry: atomic structure of newly synthesized substances
Biology: internal structure and functioning of living organisms
Geology: element and mineral (phase) composition of rocks
Ecology: quantification & speciation of industrial pollutants
Engineering: principles of operation of X-ray optical elements and detectors
History of science: bright visual experiments demonstrating basic principles and phenomena in natural science
Information technology: automation of experimental equipment, bulk data stream processing

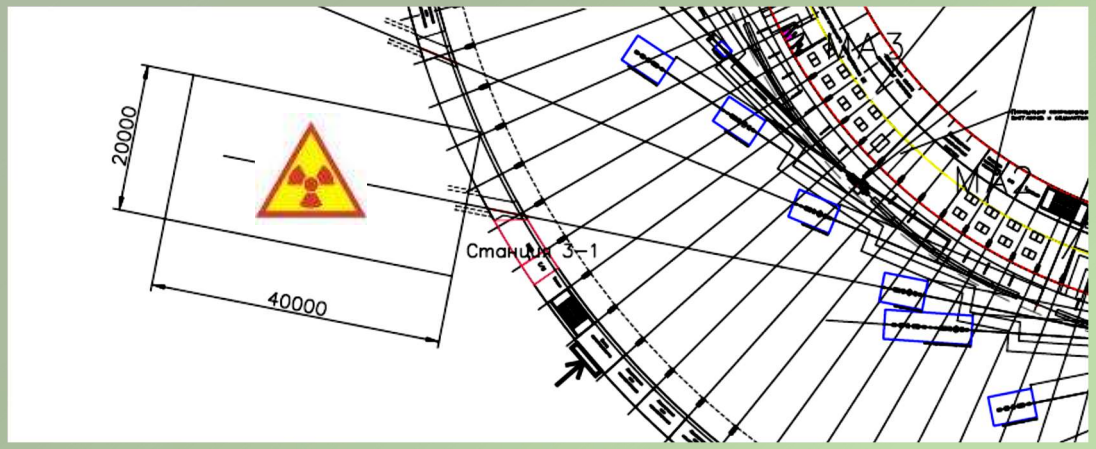


Beamline 3-1 “Isotope”

Synchrotron diagnostics of radioactive materials for solving problems related to atomic energy, nuclear medicine, and radioecology

- Novel matrices for long-term storage of spent nuclear fuel
- Efficient selective extraction of specific isotopes from nuclear waste for recycling
- Speciation of adsorption forms of transuranium elements for understanding their natural migration
- Novel radiopharmaceuticals

Separate restricted access building

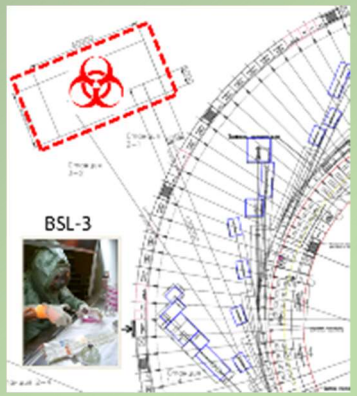


Techniques: XAFS, XRD, X-ray fluorescence analysis, to a limited extent SAXS and tomography

Design similar to BM20 (ROBL) of ESRF-EBS

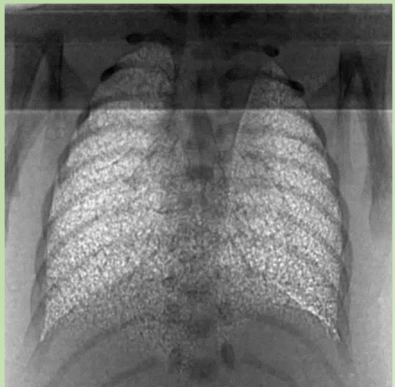
Beamline 3-2 “Vector Image” (under design in a collaboration with State Research Center of Virology and Biotechnology VECTOR)

Computed tomography of infected small (mice, rats) and medium-sized (rabbits, guinea pigs) animals with 30-50 keV photons



- Edge-enhanced absorption contrast optimized for contrasting agents containing I, Xe, Ba, Gd
- Phase contrast

Problems:
Elaboration of practical dosage forms and targeted delivery systems
Physiological response to therapeutic procedures
Comparative analysis of disease progression without and with antiviral treatment



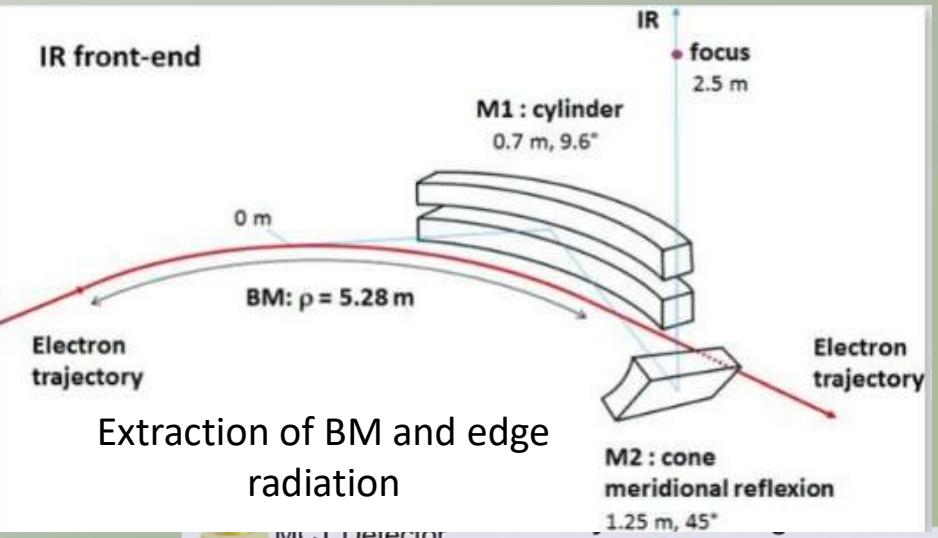
Goals:
Facile one-button operation by non-X-ray specialists
Full-field view without scanning
Real-time movie at rates coupled with physiological processes (breath, heart beating, blood circulation, etc.)
Fast-switching two-color beams for digital subtraction

Design similar to SYRMEP of Elettra

2nd phase beamlines @ LF-BMs

BL Code	Name	Source	Energy range & Techniques	Applications	Special requirements	Group
2-5	IR nanoscope	LF-BM BLA1_1L + ER from neighboring BM	sSNOM IR microscopy Magneto-Dipole spectroscopy	(Bio)polymers, carbon nanotubes, single-molecule magnets	A special photon extraction chamber with the first mirror target acceptance of 18x80 mrad² (VxH) followed by multiple periscope mirrors	Methodical development
3-13	Development (soft X-ray)	LF-BM LF-BM BLA9_1L	Metrology, feasibility studies of novel concepts 0.1-1.2 keV	In-house instrumentation development	Robust and flexible design to meet various requirements	Technology
3-14	Magneto-optics	LF-BM BLA7_1L	Resonant reflectometry near M-edges of 3d transition metals based on MOKE	In situ control of magnetic film growth	PLD/CVD-deposition unit and cryomagnetic cell included	Methodical development
3-15	Optical beam diagnostics	LF-BM BLA12_1L	E beam dynamics & emittance monitoring	Feedback with accelerator control	A fast-operating imaging detector inside frontend	Technology
3-16	Metrology	LF-BM BLA14_1L	Absolute measurements of optical constants (absorption, reflectivity, luminescence), detector sensitivity calibration 0.01-5 keV	Metrological attestation and absolute calibration in EUV, soft and tender X-ray ranges	Two replaceable sets of optical elements based on PGM and Si crystals	Technology
3-17	Control of optical elements	LF-BM BLA11_1L	Shape & roughness control, focusing performance, wave-front preservation quality 2-6 keV	Acceptance testing, in-house development of X-ray optical elements (mirrors, CRLs, multilayer structures, crystals, etc.)	A large optical table with various high-precision positioning mechanics to adopt various measurement schemes	Technology
3-18	Lithography	LF-BM	High lateral resolution lithography 0.3-6 keV High aspect ratio deep lithography 3-12 keV	Microfabrication	Two independent instruments with a common optical scheme	Technology
3-19	Flame	LF-BM	Molecular spectroscopy in the gas phase, coincidence spectroscopy (photoelectron-photoion, etc.) 0.01-0.9 keV	Studies of radical-mediated mechanisms of burning and pyrolysis processes	A special reaction gas chamber included	Methodical development

Beamline 2-5 “IR nanoscope”

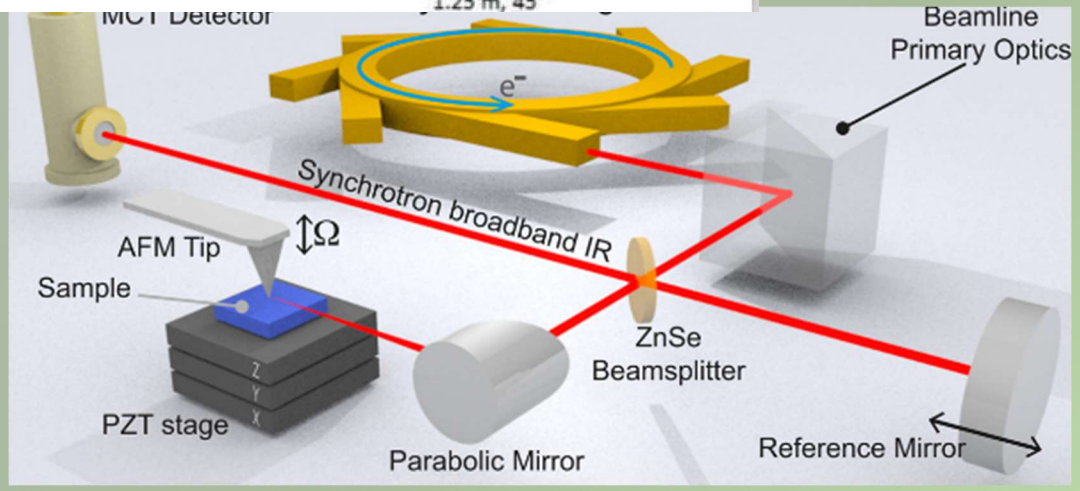


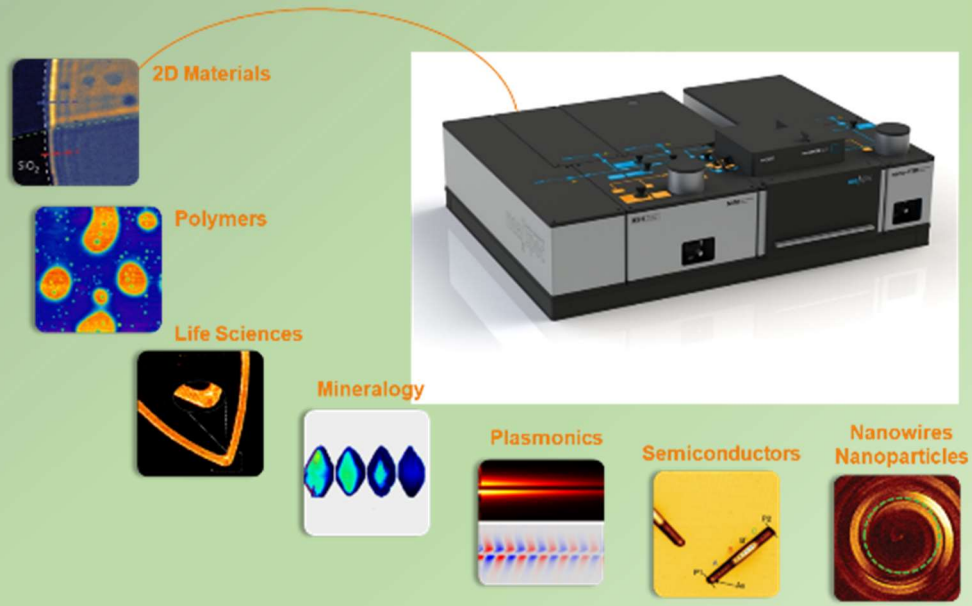
Extraction of BM and edge radiation

Techniques:

- s-SNOM
- IR spectromicroscopy
- magneto-dipole spectroscopy

Wavelength range:
ca. 2 mm – 1 μm

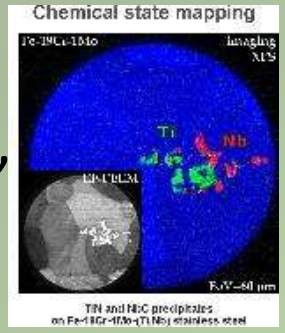




Design similar to MIRAS of ALBA, 22-IR of NLSL-II, IMBUIA of SIRIUS

Group of beamlines “Methodical development”

- **Beamline 2-5** “IR nanoscope”
- **Beamline 3-5** “Spectrum” (soft & tender spectroscopies, variable polarization)
- **Beamline 3-6** “Soft X-ray nanoscope” (water-window STXM and PEEM)
- **Beamline** 3-7 “Gamma-2” (Mössbauer of exotic nuclei)
- **Beamline 3-11 “**Surface” (real-time monitoring of thin film formation via ion plasma deposition using GI-XRD, GI-SAXS, X-ray reflectivity, and CTR)
- **Beamline 3-14** “Magneto-optics” (Ultrasoft reflectivity, T-MOKE effect)
- **Beamline 3-19** “Flame” (Molecular spectroscopy of burning and pyrolysis products in EUV & Ultrasoft ranges)



Group of beamlines “Uninterrupted operation”

Beamline 3-3 “Protein” (MX)

Beamline 3-9 “Single crystal” (small-molecule Xtal)

Beamline 3-8 “SAXS”

Beamline 3-9 “XAFS”

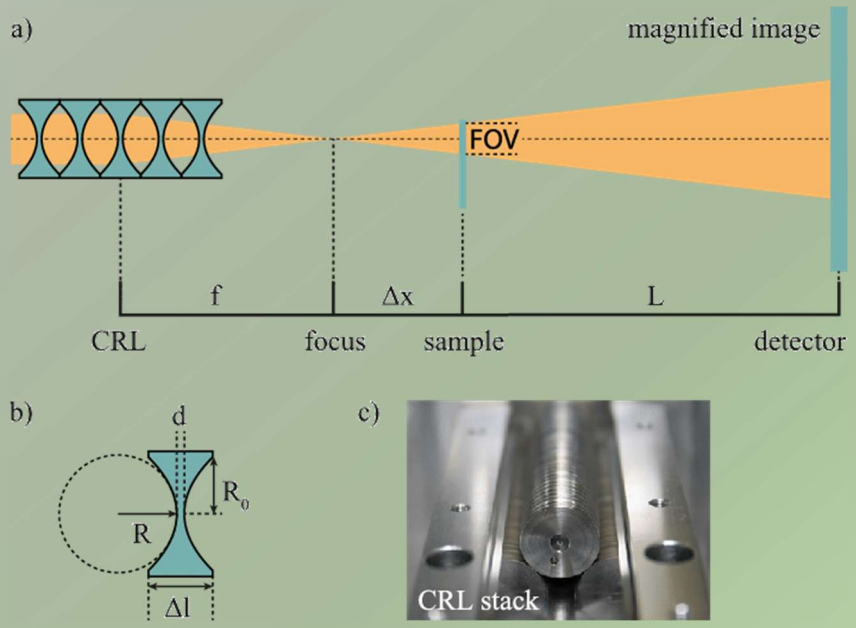
Beamline 3-10 “High-precision X-ray crystallography” (small-molecule Xtal)

Group of beamlines “Technology”

Beamlines 3-12, 3-13 *In-house instrumental development and testing*

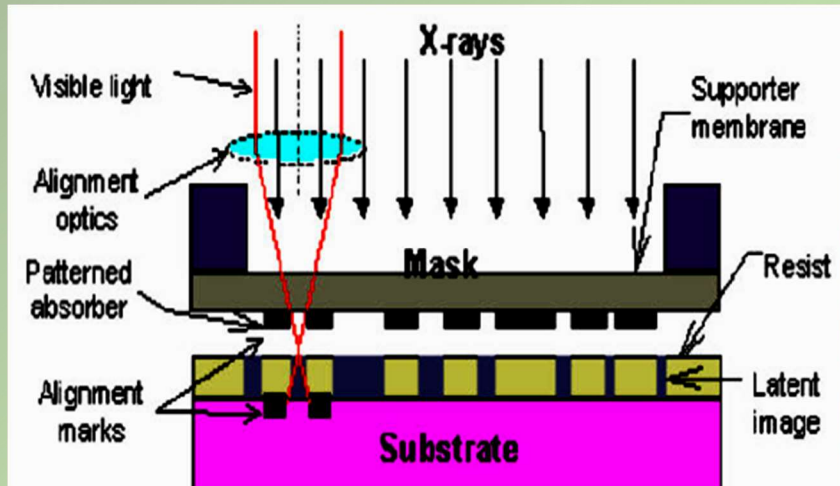
Beamline 3-15 *Real-time e-beam optical diagnostics*

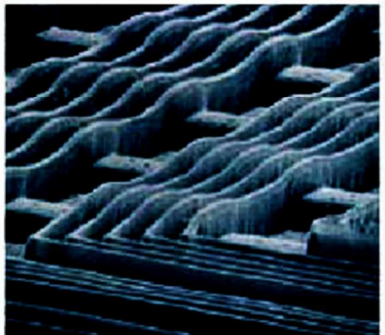
Beamline 3-16 *Metrology (absolute calibration of detectors over wide spectral range)*



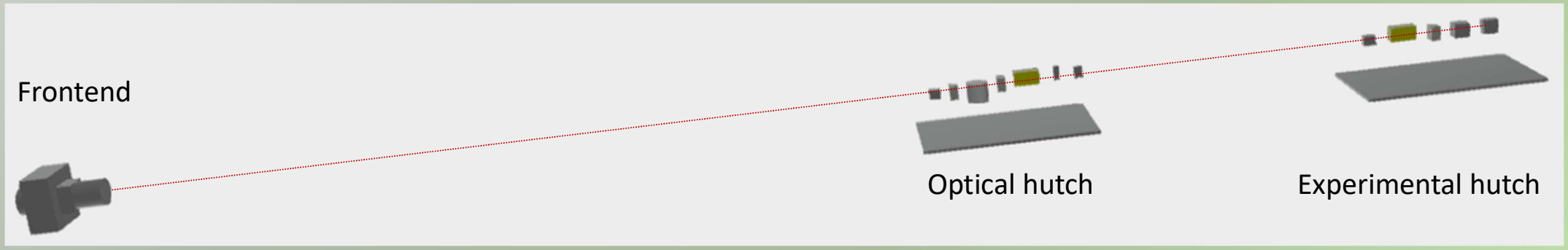
Beamline 3-17 *Control of optical elements (shape & roughness, focusing performance, rocking curves, dislocation density, etc.)*

Beamline 3-18 *X-ray lithography (high-lateral-resolution @ 0.3-6 keV and deep high-aspect-ratio @ 3-12 keV)*





Default configuration



Typical length of optical scheme ~60 m (~30 m downstream to frontend)

Engineering infrastructure
- Compressed air
- Dry N_2
- Deionized cooling water

Nominal electrical power ~55 kW

Optical hutch 6×4 m^2 (35 m from the source)

- Frontend exit window
- Entrance slits
- Beam position monitor
- Monochromator
- Beam position & intensity monitor
- Focusing element (mirror or CRL)
- Monochromatic beam shutter
- Bremsstrahlung stop

All elements are on bulky granite base blocks to suppress vibrations

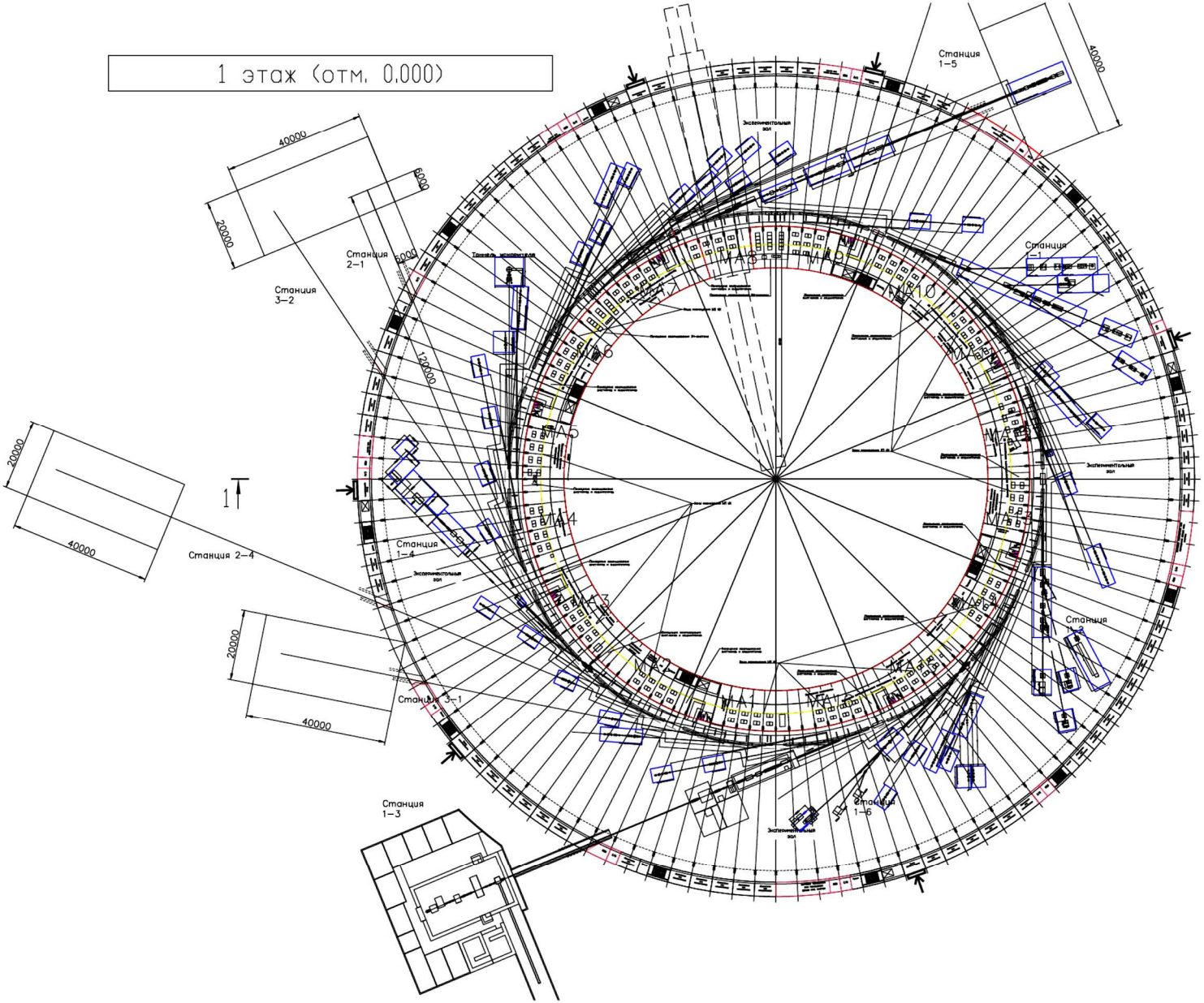
Experimental hutch 6×4 m^2 (55 m from the source)

- Beam-forming slits
- Final focus lens
- Beam position & intensity monitor
- Sample stage
- Detector system

All elements are on a common optical table

General scheme:

Main accelerator building and satellite buildings



Conclusions & Outlook

- The list of 2nd-phase beamlines is still under discussion and reconciliation
- Many beamline teams are in the premature state
- New ideas and recommendations are cordially welcome!

ИНХ СО РАН

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РФЯЦ-ВНИИТФ

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