BORESKOV INSTITUTE OF CATALYSIS

СКИФ

The design of «Structural Diagnostics» beamline for SRF «SKIF»

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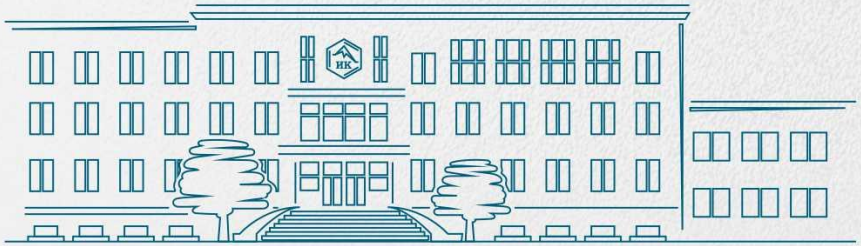


Novosibirsk, 2020

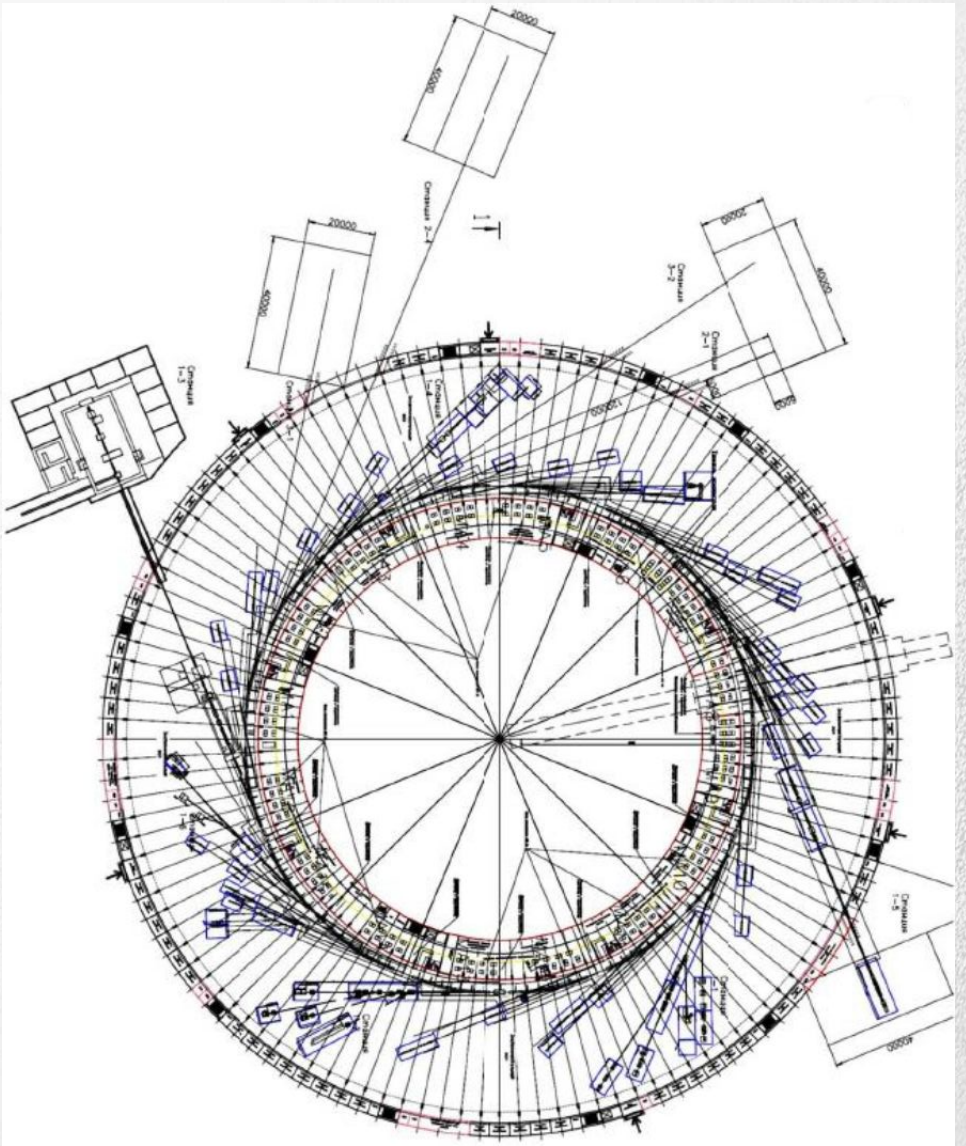
SRF “SKIF” – Shared Research Facility, Siberian Circular Photon Source

Project is initiated by a special Order of Vladimir Putin, President of RF.

The first stage of the project is to be finalized in 2024. Location – Novosibirsk District, Koltsovo.

Parameter	Value
Energy	3 GeV
Current	Up to 400 mA (2 mA in a bunch)
Emittance	90 pm·rad
Injection type	Full injection
Circumference	476 m
Number of experimental stations	6 (first phase) +24 (second phase)
Number of IDs	14

Main view of SRF “SKIF”, 1st phase and future beamlines



1st phase beamlines:

1-1 “MicroFocus”

1-2 “Structural Diagnostics”

1-3 “Fast Processes”

1-4 “XAFS and MCD”

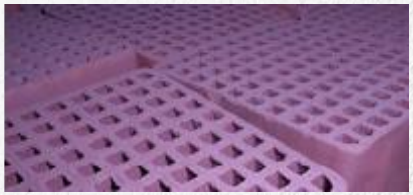
1-5 “High-energy X-ray diagnostics”

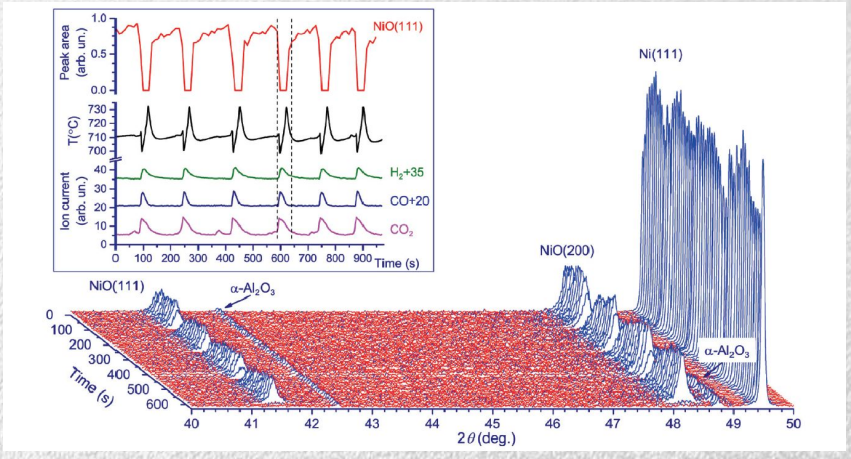
1-6 “Electronic structure”

Application of X-ray diffraction techniques to solve a wide range of research and technological problems

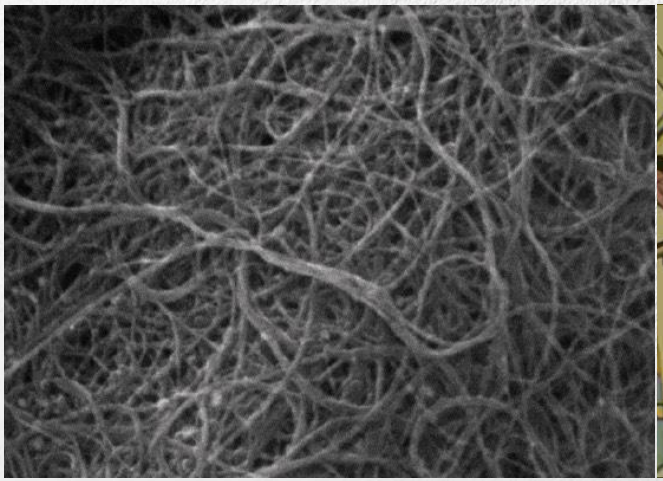
Scientific Scope Overview

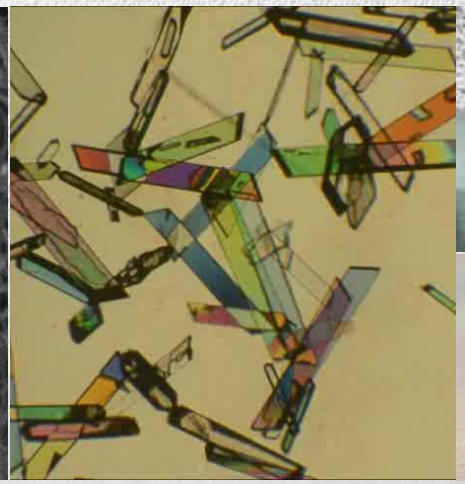
Hydrogen Energy, Fuel Cells, Catalysis, Ceramics and Films, Disordered Materials

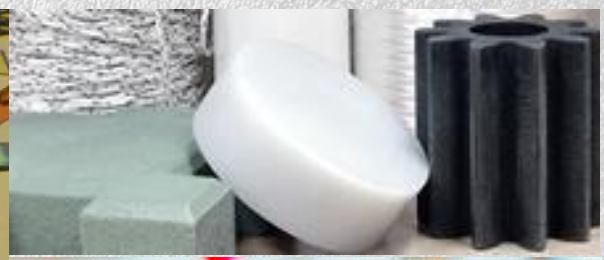




Polymer and Carbon Materials, Dispersed Phases, Nanomaterials, Pharmaceuticals, Single crystals







“Structural Diagnostics” Beamline

Application of X-ray diffraction techniques to a wide range of research and technological problems

Beamline 1-2

“Structural Diagnostics”

High-res

High-resolution X-ray diffraction techniques at variable energies of SR

SC-XRD

Single-crystal X-ray diffraction for the samples which are not suitable for conventional laboratory diffractometers (studying processes, small size, unstable samples *etc.*)

In Situ

In Situ and *Operando* studies at high temperatures and in variable gas atmospheres, including catalytic processes and chemical reactions

SAXS

SAXS for wide range of objects including biological samples, inorganic materials *etc.*

Research Directions and Sections of the Beamline

(1) Section «High resolution X-ray diffraction» (Primary section) (2) Section «Single-crystal X-ray diffraction» (3) Section «*In Situ* studies at high temperatures and in gas environment» (4) Section «Small-angle X-ray scattering»	(1)	(2)	(3)	(4)
Unit 1 «Materials for hydrogen energy and fuel cells»				
Unit 2 «Catalysts for energy efficient catalysis, oil refining and ecology applications»				
Unit 3 «Ceramics and energetic materials»				
Unit 4 «Films and membranes»				
Unit 5 «Systems with partially disordered hierarchical structure: polymers and carbon materials»				
Unit 6 «Pharmaceuticals and biomaterials»				
Unit 7 «Single crystals»				
Unit 8 «Structural diagnostics of highly-disperse and nanostructured systems»				

Source

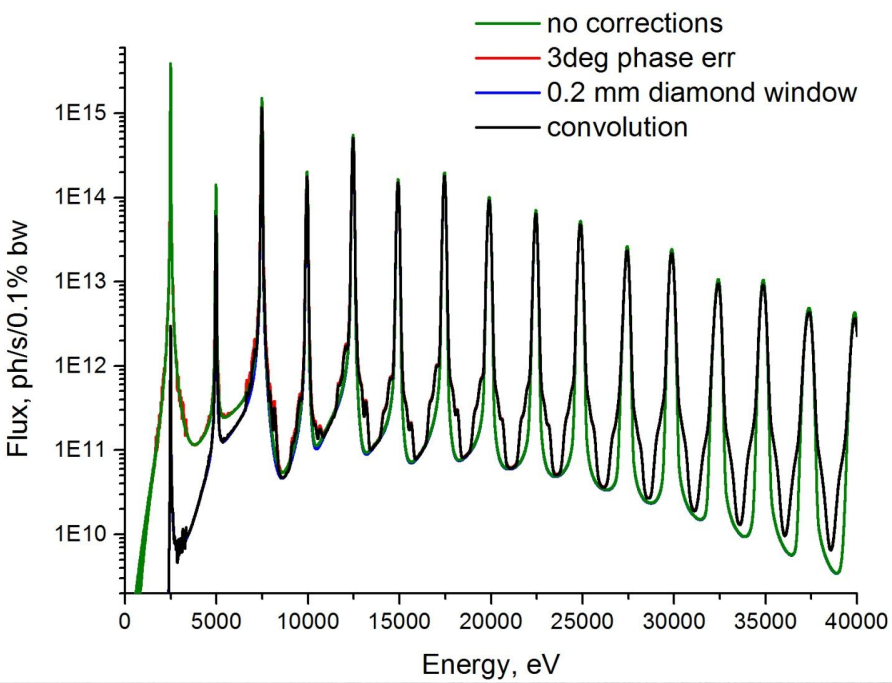
SC undulator, main mode: B = 1.06 T, K = 1.54 (B_{max} – 1.2 T)

Period, mm	15.6
Length, m	2
No of periods	128

Gap, mm	6
B_{max}, T	1.2
K_{max}	1.75

B error < 0.1 %, phase error < 3°

Flux on 1 x 1 mm^2 at 26 m from the source



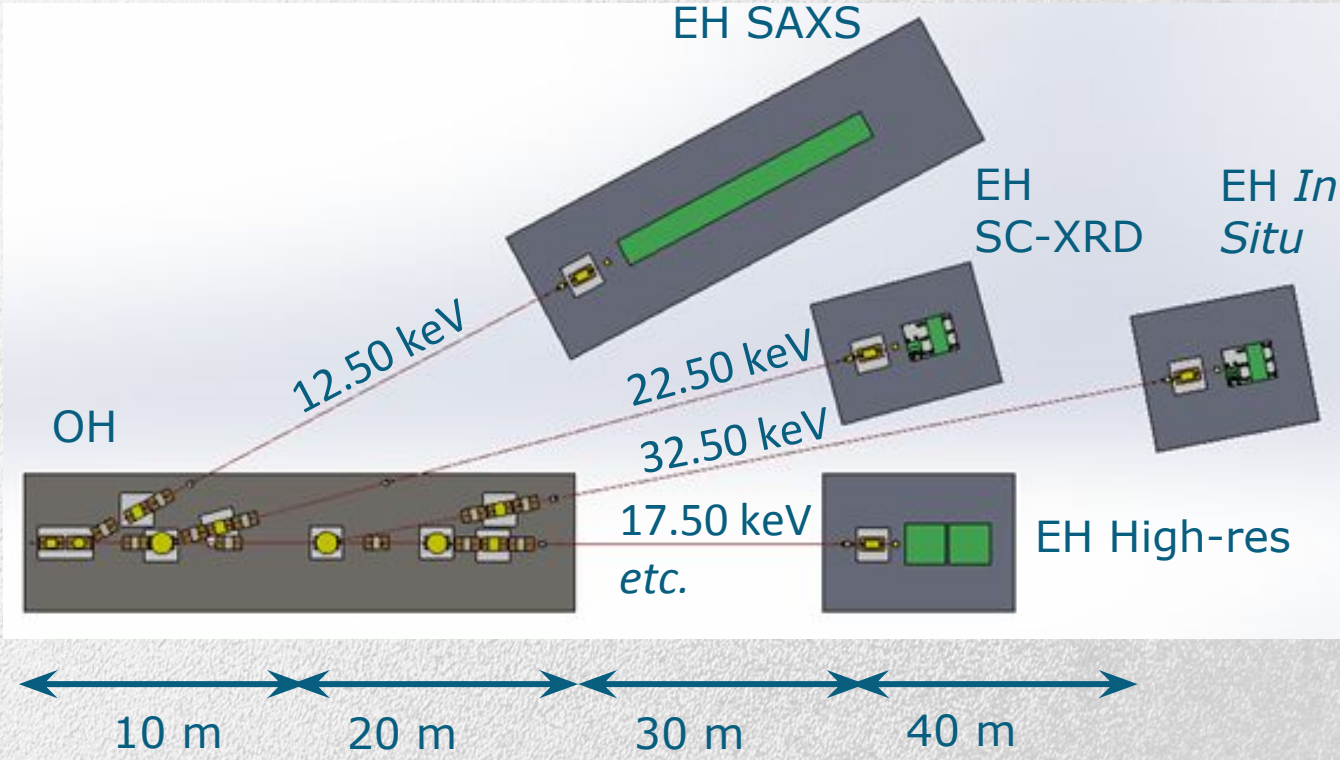
Harmonics energies in main mode

Harmonics	Energy, keV	λ, Å	Section
1	2.5	4.96	-
3	7.5	1.65	High-res
5	12.5	0.99	SAXS
7	17.5	0.71	High-res
9	22.5	0.55	SC-XRD (SM Xtal)
11	27.5	0.45	High-res
13	32.5	0.38	In Situ (XRD)

Optics concept

Diamond (111) beam splitters are used to deliver 5th (12.50 keV / 0.99 Å), 9th (22.50 keV / 0.55 Å) and 13th (32.50 keV / 0.38 Å) harmonics to side sections + DCM Si(111) for straight section

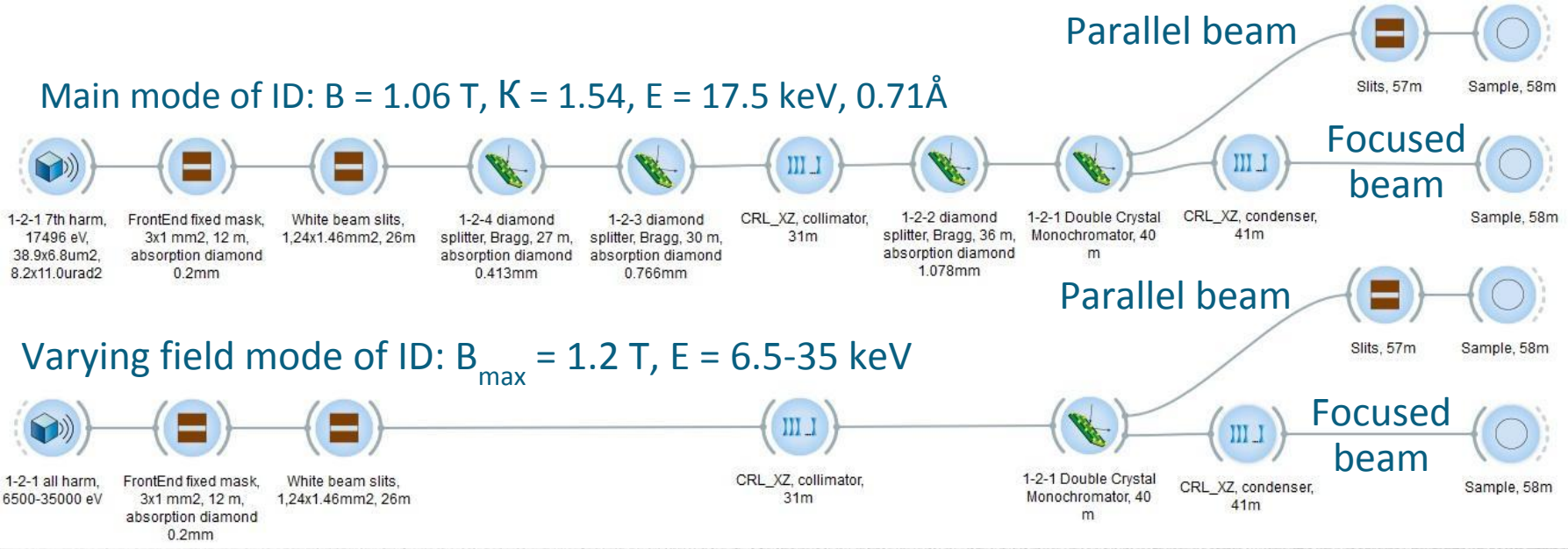
Green – diffractometers, **yellow** – diamond beam splitters, DCM and CRLs (control rooms are not shown)

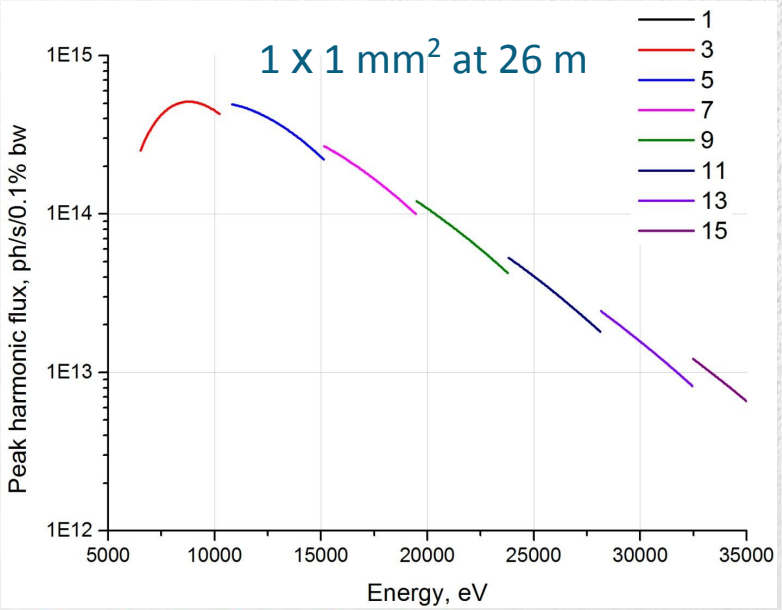


Features:

- Simultaneous operation of all sections in main mode (fixed energy)
- Alternative mode with ID tuning (side sections are out of operation, continuous energy variation)

High resolution X-ray diffraction (High-res, Primary section)



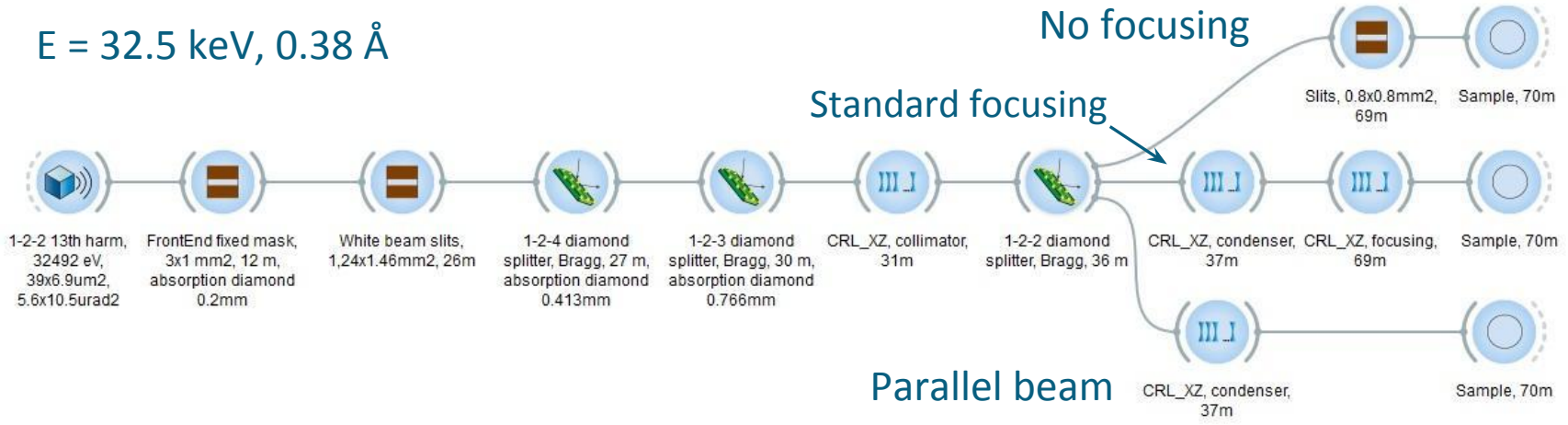


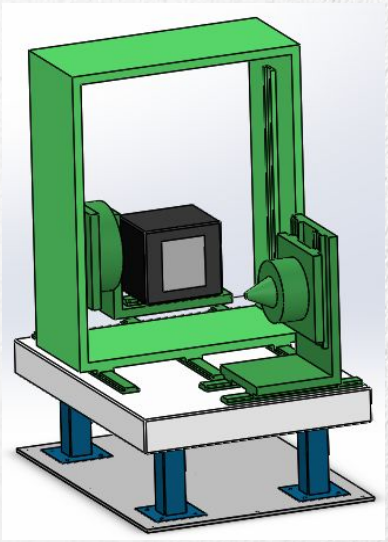
2D parabolic CRLs, curvature radius 500 µm

Number of Be lenses in CRL units 1 & 2, CRL1 (31m), CRL2 (41m)	Beam size, FWHM², µm²	Flux, ph/s, (% of unfocused beam)	Flux density, ph/s/mm²	Resolution at 30°, FWHM, °
7, 13	50×24	9.4×10^{12} (72%)	8.9×10^{15}	0.0033
7, 0	571×667	1.1×10^{13} (85%)	2.9×10^{13}	0.0026
0, 0	1100× 1440	1.3×10^{13} (100%)	8.0×10^{12}	0.0047

In Situ studies at high temperatures and in gas environment (*In Situ*, side section, fixed E)

E = 32.5 keV, 0.38 Å





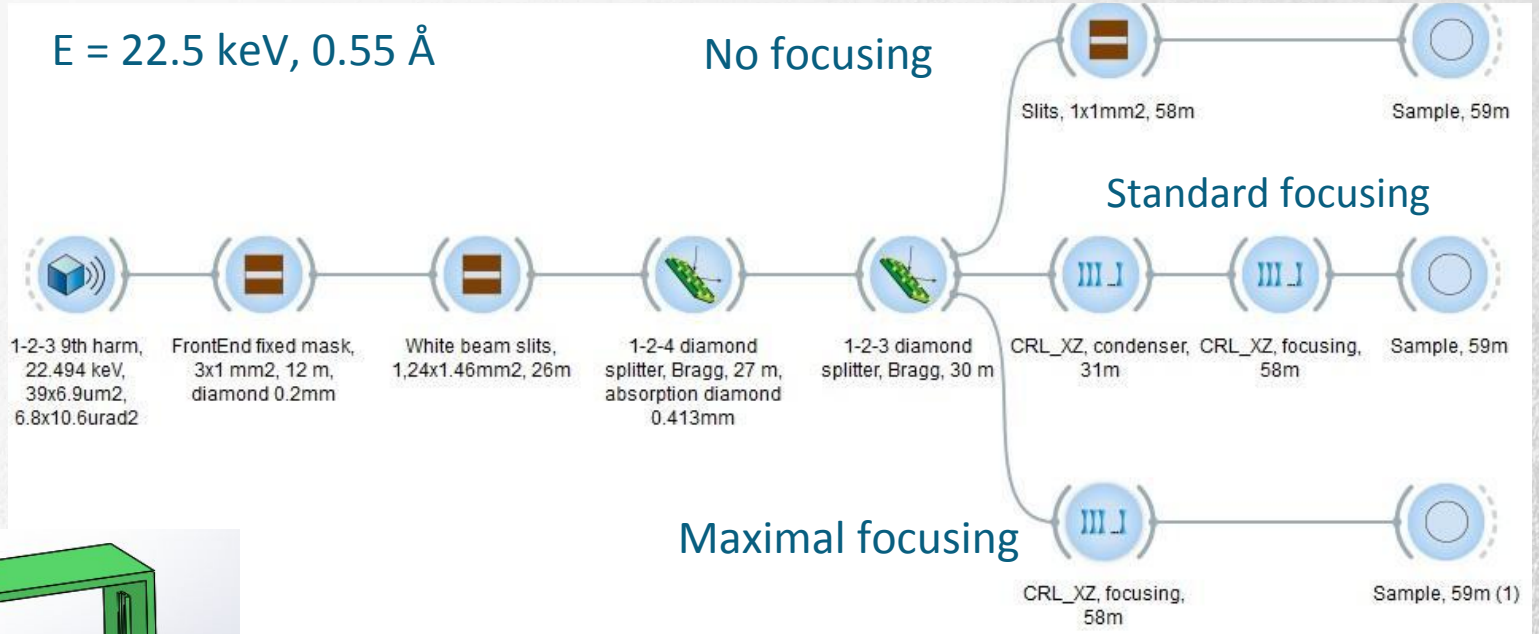
+ Dectris PILATUS 3X CdTe 2M

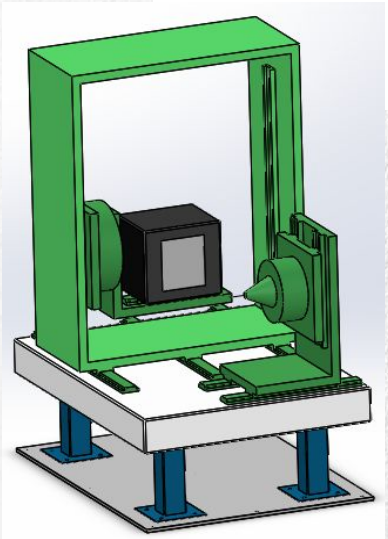
Number of Be lenses in CRL units, CRL1_XZ_R500 (37m, 2D) CRL1_Z_R500 (37m, 1D) CRL2_XZ_R50 (68m, 2D) CRL2_X_R200 (68m, 1D)	Beam size, FWHM^2, µm^2	Flux, ph/s, (% of unfocused beam)	Flux density, ph/s/mm^2	Divergence at sample position, FWHM, mrad^2
22, 6, 30, 10	7.8×6.2	1.7×10^{11}(44%)	3.5×10^{15}	0.09×0.1
0, 10, 0, 0	685×910	3.6×10^{11}(92%)	5.8×10^{11}	0.007×0.005

Key features & accessories: hard energy, reaction chambers and high-temperature devices, gas supply and mass-spectrometer

Dyadkin V., Pattison P., Dmitriev V., Chernyshov D. A new multipurpose diffractometer PILATUS@SNBL // J. Synchrotron Rad. 2016. Vol. 23, № 3. P. 825–829

Single-crystal X-ray diffraction (SC-XRD, side section, fixed E)





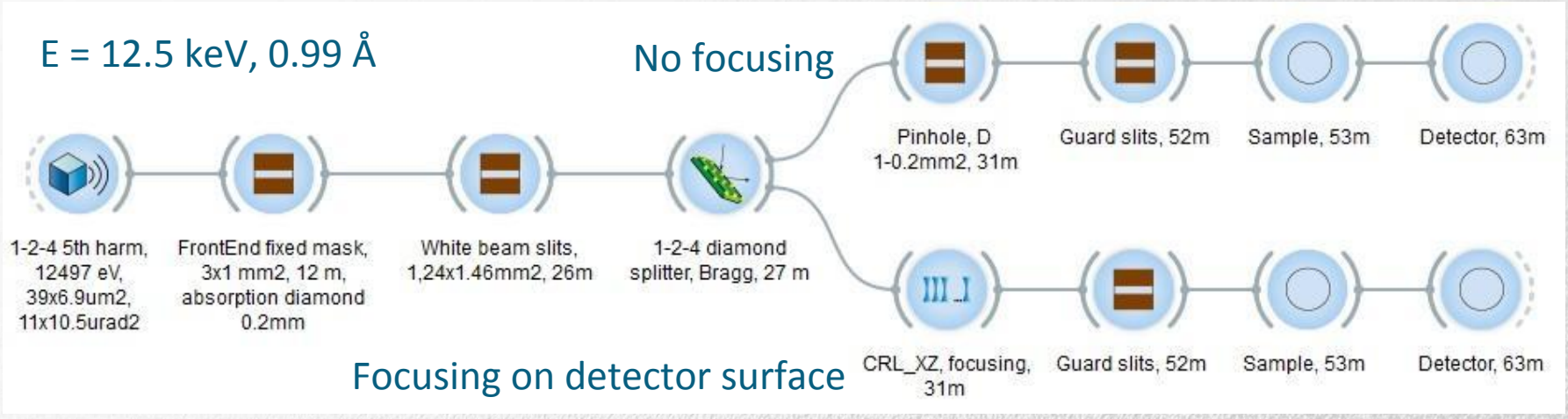
+ Dectris PILATUS 3X CdTe 2M

Number of Be lenses in CRL units, CRL1_XZ_R500 (31m, 2D) CRL1_Z_R500 (31m, 1D) CRL2_XZ_R50 (58m, 2D) CRL2_X_R200 (58m, 1D)	Beam size, FWHM^2, μm^2	Flux, ph/s, (% of unfocused beam)	Flux density, ph/s/mm^2	Divergence at sample position, FWHM, mrad^2
0, 0, 75, 1	0.82×0.81	10^{11}(3%)	1.6×10^{17}	0.4×0.4
2, 7, 0, 0	838×855 (10×10- min)	2.7×10^{12}(90%)	3.7×10^{12}	0.0013×0.006

Dyadkin V., Pattison P., Dmitriev V., Chernyshov D. A new multipurpose diffractometer PILATUS@SNBL // J. Synchrotron Rad. 2016. Vol. 23, № 3. P. 825–829

Key accessories: κ-goniometer, cryostream cooler and stream heater, online Raman spectrometer (pressure measurement, sample control)

Small-angle X-ray scattering (SAXS, side section, fixed E)



Diffractometer solution from XENOCS (Xeuss 3.0 diffractometer, 10 m length, Dectris Eiger2 X 4M for SAXS + Dectris Pulatus3 X 100K-M WAXS detector)

Focused (28 m, 27 lenses CRL1_XZ_R2000, 1 lense CRL1_X_R2000)					
1st aperture diameter, mm	2nd aperture diameter, mm	Beam size, FWHM², μm²	Flux, ph/s, (% from unfocused beam)	Flux density, ph/s/mm²	Q_{min}, Å^{-1}
0.2	0.096	70×68	8.7×10^{11} (3%)	1.8×10^{13}	1.5×10^{-4}
1	0.35	232×239	1.1×10^{13} (42%)	2.0×10^{14}	6.1×10^{-4}
1.5	0.5	268×287	1.7×10^{13} (65%)	2.2×10^{14}	9.0×10^{-4}
Unfocused					
0.5	0.87	660×690	6.3×10^{12} (24%)	1.4×10^{13}	1.0×10^{-3}
1	1.7	1140×1140	1.8×10^{13} (69%)	1.4×10^{13}	2.0×10^{-3}

Key accessories: GISAXS module, automatic sample changer, chambers for in situ experiments under controlled T, P and gas atmospheres

Summary

-A wide range of diffraction studies can be performed at the beamline with the conceptual design presented to solve research and (or) technological tasks;

-Powder XRD, single-crystal XRD and SAXS techniques will be available including *in situ* experiments at variable T, P and gas environments;

-High intensity and low initial divergence of the beam allow one to control beam size and divergence at the sample positions by refractive X-ray optics and perform experiments either with bulk and small samples or mapping experiments.

Thank you for your kind attention!

Announcement

1) … more information on “Structural Diagnostics” beamline optics:

Zakhar S. Vinokurov *et al.*

(Poster 10)

Optical design of the «Structural Diagnostics» beamline for SRF «SKIF»

2) Special Session on SKIF Project:

(16-07-2020, Start at 14-00)

General session on SKIF Project

Thank you for your kind attention!

Novosibirsk District, September 2018