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

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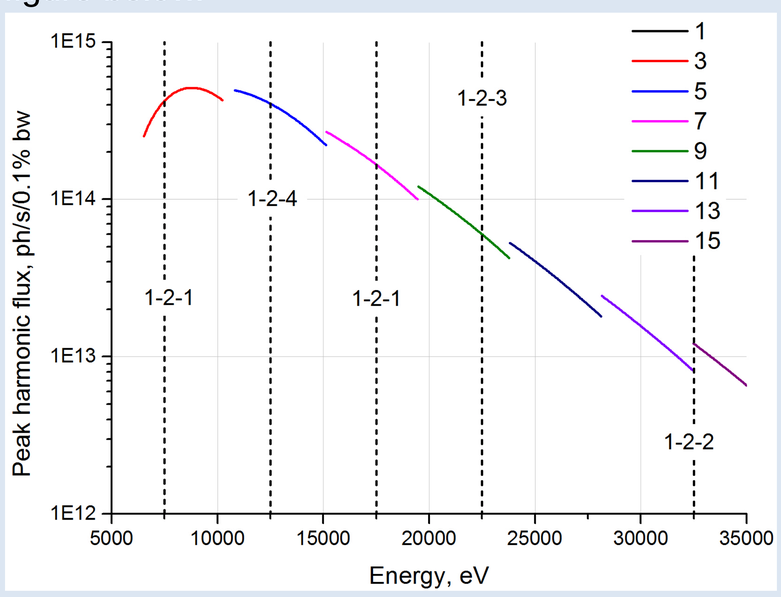
Scientific scope

Application of X-ray diffraction techniques to a wide range of research and technological problems. Beamline **1-2 "Structural Diagnostics"** includes four sections:
High-resolution powder diffraction (straight section **1-2-1 "High-res"**) – high-resolution X-ray diffraction and anomalous scattering techniques at variable energies of SR;
In situ diffraction (side branch **1-2-2 "In Situ"**) – *In Situ* and *Operando* studies at high temperatures and in variable gas atmospheres, including catalytic processes and chemical reactions;
Single-crystal X-ray diffraction (side branch **1-2-3 "SC-XRD"**) – Single-crystal X-ray diffraction for the samples which are not suitable for conventional laboratory diffractometers (small size, unstable samples *etc*.);
Small angle X-ray scattering (side branch **1-2-4 "SAXS"**) – SAXS techniques for wide range of objects including biological samples, inorganic materials *etc*.

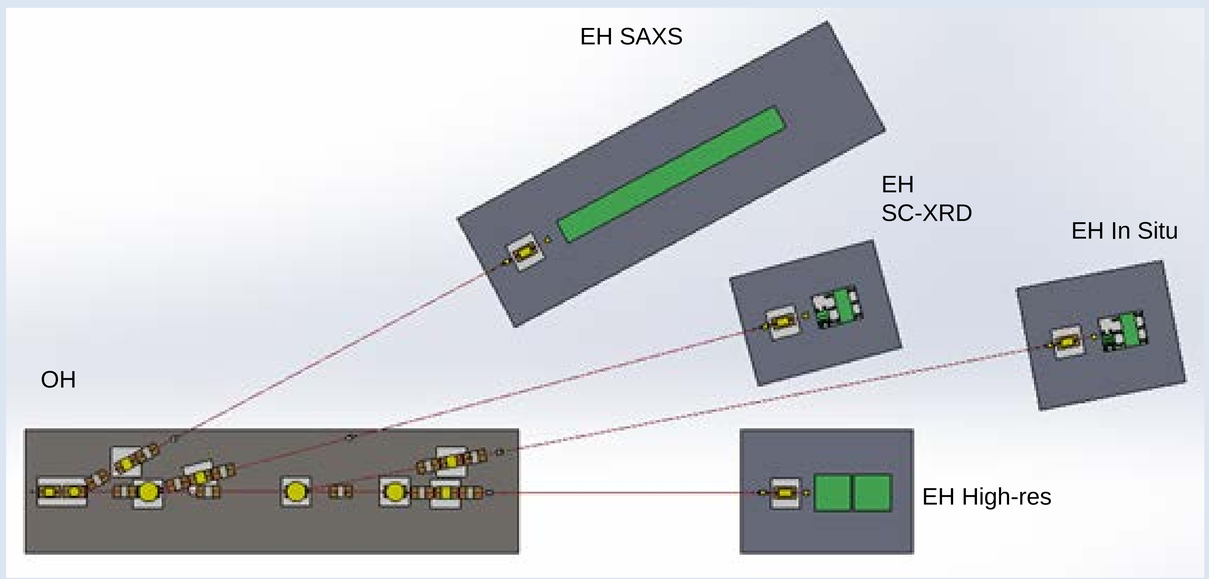
Beamline setup. Insertion Device.

A an in-vacuum superconducting undulator (SCU) insertion device is chosen to provide the x-rays with desired characteristics for the beamline. The 2 m device has an array of 128 magnets with a period length of 15.6 mm. SCU designed to produce x-rays ranging from 6.5 to 35 keV. The theoretical tuning curve of flux density for the SCU device is shown in figure below.



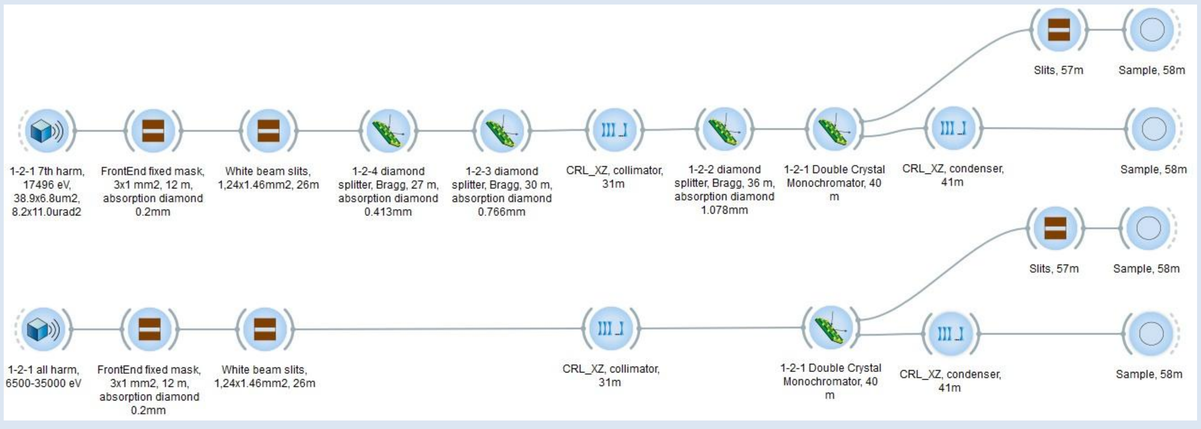
Undulator theoretical spectrum of SCU showing the first eight odd harmonics. The black dashed lines indicate the operation energy of all endstations in the primary mode (fixed energy). The solid lines shows tunable energy for the 1-2-1 straight section in the alternative mode (all side branches are off).

At the beamline **1-2 "Structural Diagnostics"**, it is planned to install three diamond monochromator crystals. Plane-parallel plates with an orientation of (111) and a thickness of about 100 μm branch off the 5th (12.50 keV / 0.99 Å), 9th (22.50 keV / 0.55 Å) and the 13th (32.50 keV / 0.38 Å) harmonics to the side branches at angles of 28, 15 and 11 °, respectively (figure below). The main advantage of such a scheme is the simultaneous and independent operation for all four instruments in the primary operating mode. The disadvantage of this approach is the fixed beam energy on the side branches.

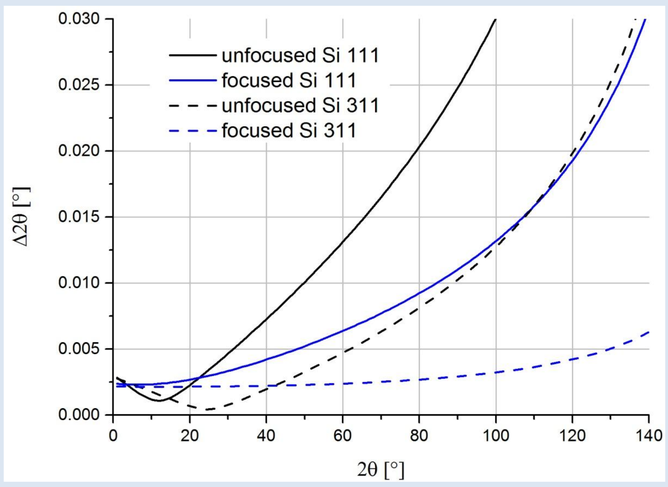


Beamline 1-2 setup, top view. Only optical (OH) and experimental (EH) hutches have shown. Optical elements (CRL's, monocromators, slits *etc.*) – yellow, endstations – green, granite bases – white.

1-2-1



Optical scheme with the major optical elements of beamline 1-2-1 and the distances to the undulator source. Two branches shows two modes of operation (primary and with energy tuning).



Theoretical curves of the instrumental resolution function for 1-2-1 working in the high-resolution mode at an energy of 17.5 keV when using Si (111) and Si (311) crystals (monocromator and analyser). Blue lines - with collimating (31 m) and focusing (41 m) CRL's, black - without focusing.

Beam characteristics at the sample position for various focusing options (monochromator and analyzer Si (111) crystals) in a high-resolution mode.

CRL's quantity, CRL1_XZ_R500 (31m, 2D parabolic, curvature radius 500 μm), CRL2_XZ_R500 (41m)	Beam size, FWHM^2, μm^2	Flux, ph/s, (% from unfocused beam)	Flux density, ph/s/mm^2	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

1-2-2, 1-2-3, 1-2-4

Beam characteristics at the sample position for various focusing options (1-2-2 branch).

CRL's quantity, 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, (% from 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

Beam characteristics at the sample position for various focusing options (1-2-3 branch).

CRL's quantity, 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, (% from 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	2.7×10^{12}(90%)	3.7×10^{12}	0.0013×0.006

Beam characteristics at the sample position for various focusing options (1-2-4 branch).

Focused (28 м, 27 CRL1_XZ_R2000, 1 CRL1_X_R2000)					
1st aperture diameter, mm	2nd apperture diameter, mm	Beam size, FWHM^2, μm^2	Flux, ph/s, (% from unfocused beam)	Flux density, ph/s/mm^2	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}

Acknowledgements

The work was supported by Ministry of Science and Higher Education of the Russian Federation (grant No. AAAA-A19-119020890025-3).
Theoretical parameters were calculated using the SPECTRA [1] and SHADOWOUI [2].

[1] Tanaka T. Universal representation of undulator phase errors // Physical Review Accelerators and Beams. 2018. Vol. 21, № 11. P. 110704.
[2] Rebuffi L., Sánchez del Río M. ShadowOui : a new visual environment for X-ray optics and synchrotron beamline simulations // Journal of Synchrotron Radiation. 2016. Vol. 23, № 6. P. 1357–1367.